Development of nuclear data processing code FRENDY

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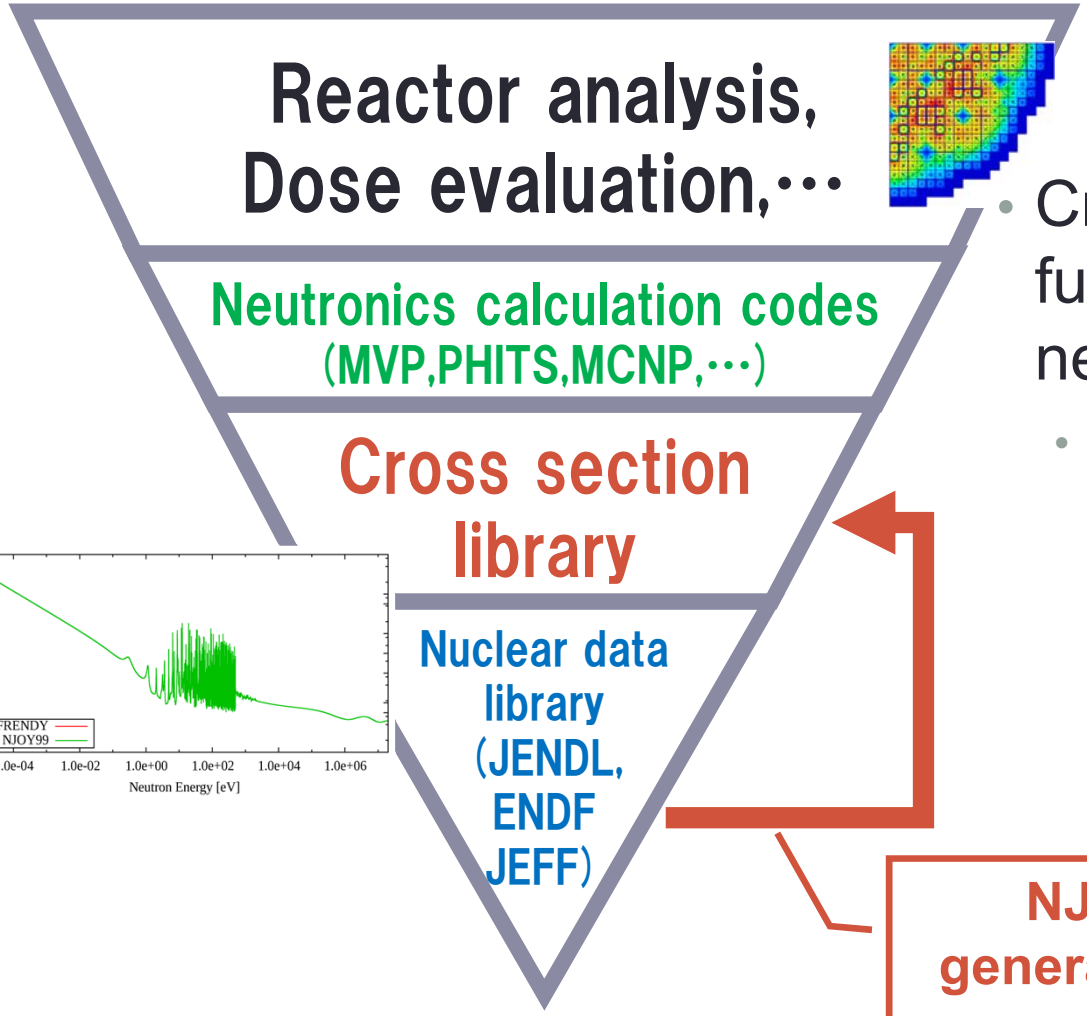
Outline

- Overview of nuclear data processing
- Overview of FRENDY
  - Nuclear data processing codes development in the world
  - Collaboration with international organizations
- Comparison of processing results between FRENDY and NJOY
- Conclusions

Overview of nuclear data processing and FRENDY

Importance of nuclear data processing

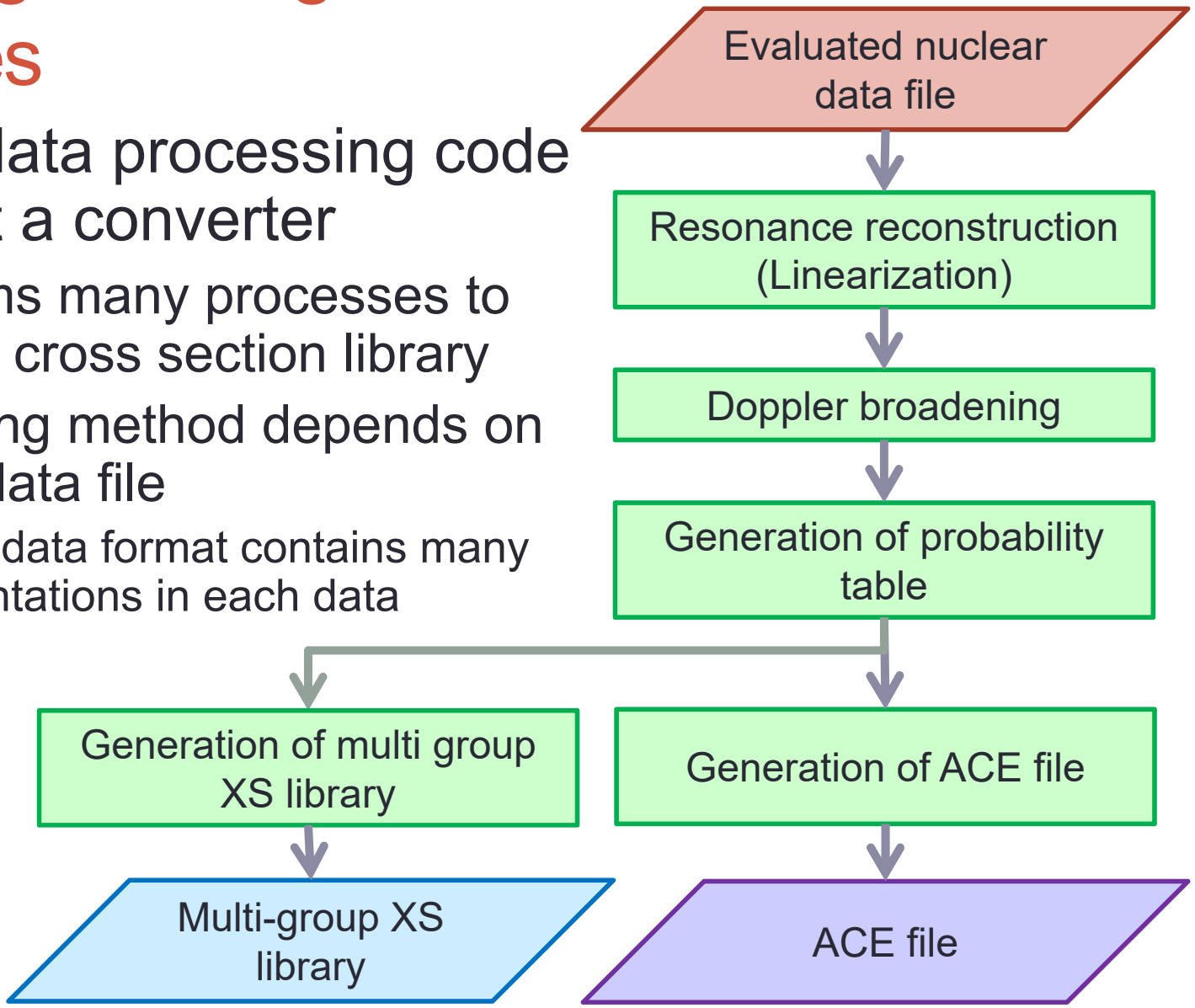


- Cross section library is the fundamental data for the neutronics calculations
  - Reliability of the cross section library has large impact on the neutronics calculation

NJOY is widely used to generate cross section library in Japan

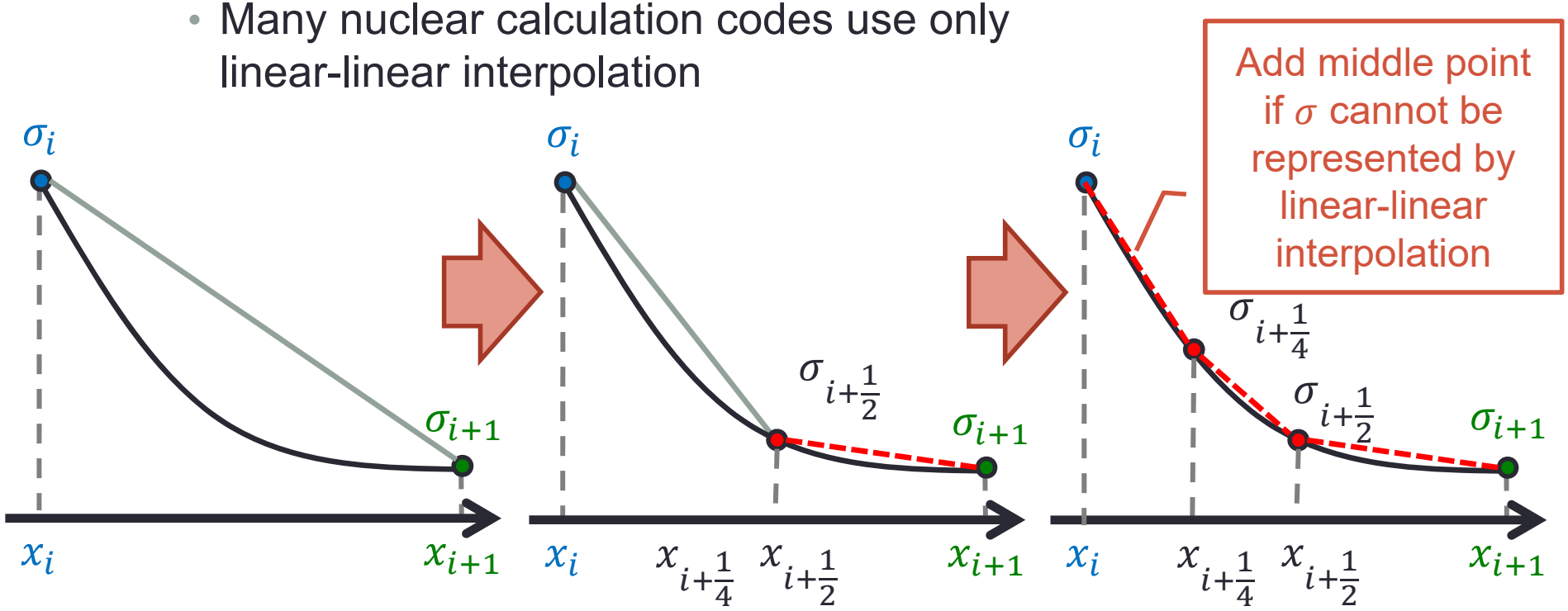
Processing flow to generate XS libraries

- Nuclear data processing code is not just a converter
  - It performs many processes to generate cross section library
  - Processing method depends on nuclear data file
    - Nuclear data format contains many representations in each data



Linearization

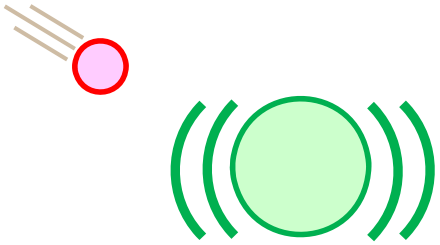
- Evaluated nuclear data library describes cross sections with different interpolation scheme
  - Log-log interpolation, linear-linear interpolation, …
  - Different interpolation schemes are inconvenient
    - Linearization is required for Doppler broadening
    - Many nuclear calculation codes use only linear-linear interpolation



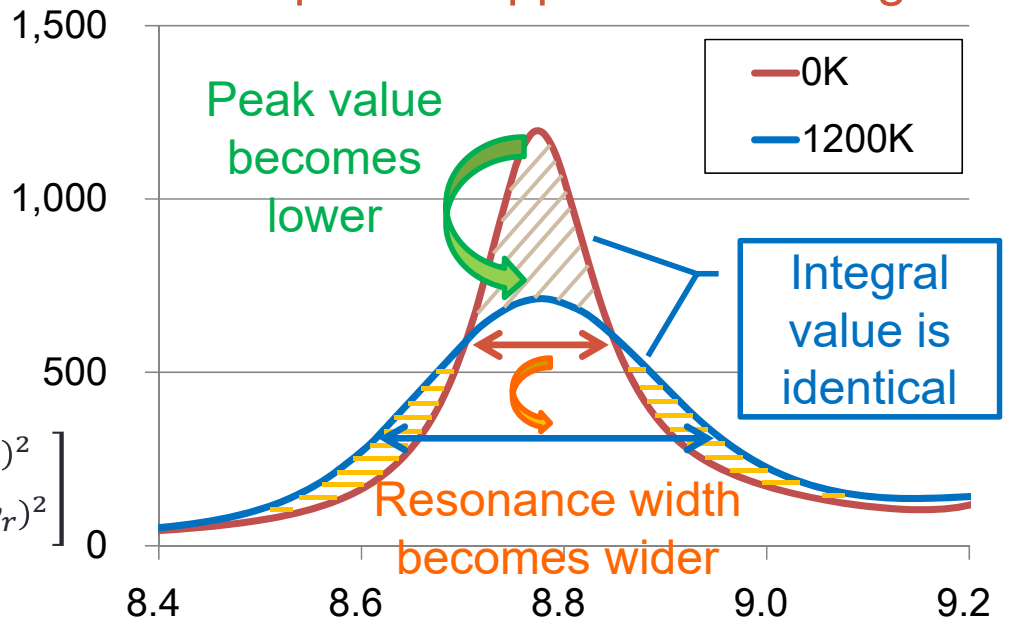
Doppler broadening

- Most of evaluated nuclear data files contain cross sections at 0 K
  - Consideration of nucleus vibrates (Doppler broadening) are required to calculate cross section at T K

【Reaction of incident particle and nucleus】



【Example of Doppler broadening】



【Equation of Doppler broadening】

$$\sigma(v,T)=\frac{1}{v^2}\sqrt{\frac{\beta}{\pi}}\int_0^{\infty}dv_r v_r{}^2\sigma(v_r)\left[\begin{matrix}e^{-\beta(v-v_r)^2}\\-e^{-\beta(v+v_r)^2}\end{matrix}\right]$$

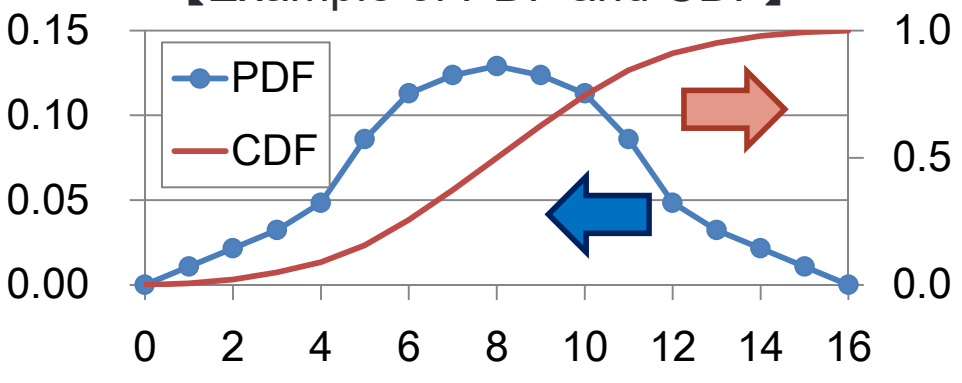
T: Temperature,

v: velocity of incident particle, v_r: relative velocity

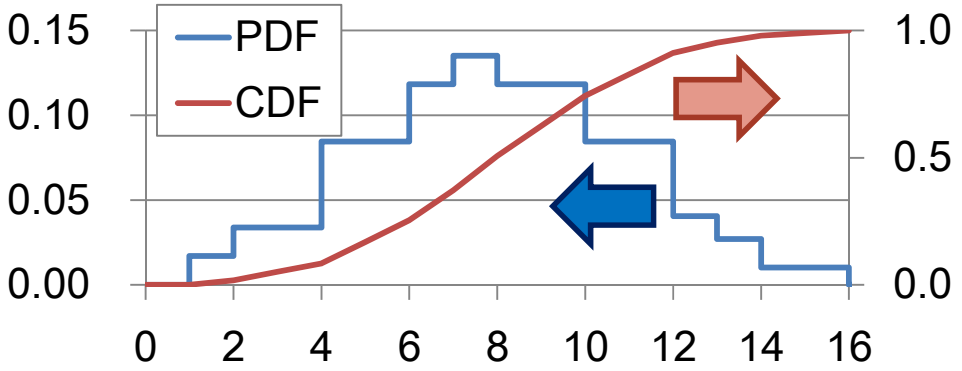
Generation of ACE file

- Continuous energy Monte Carlo calculation codes use cumulative probability distribution (PDF/CDF)
  - Cross section, angular and energy distributions are converted to cumulative probability distribution
  - PDF: Probability Density Function
  - CDF : Cumulative Density Function

【Example of PDF and CDF】



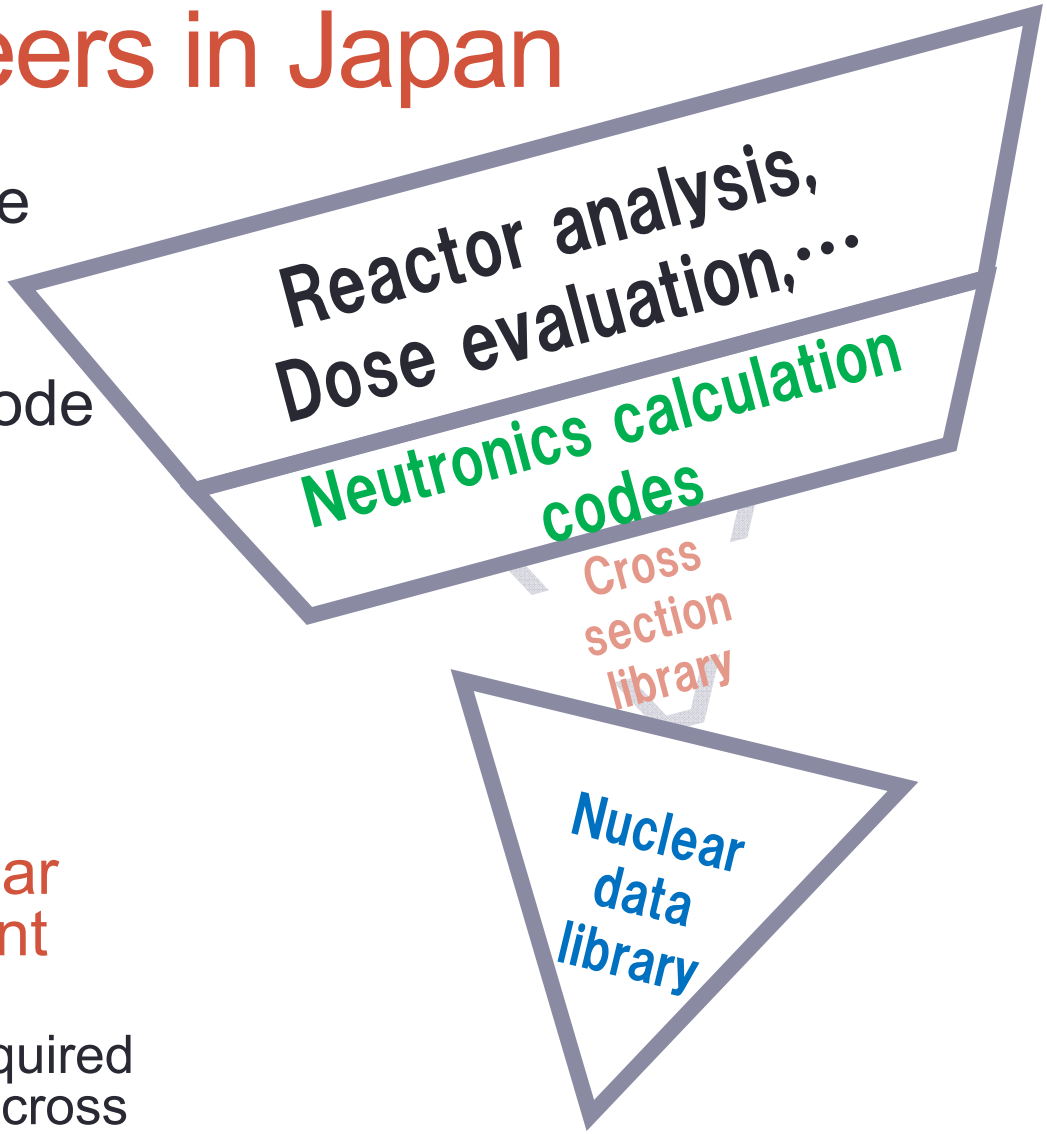
From linear-linear to PDF/CDF



From histogram to PDF/CDF

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

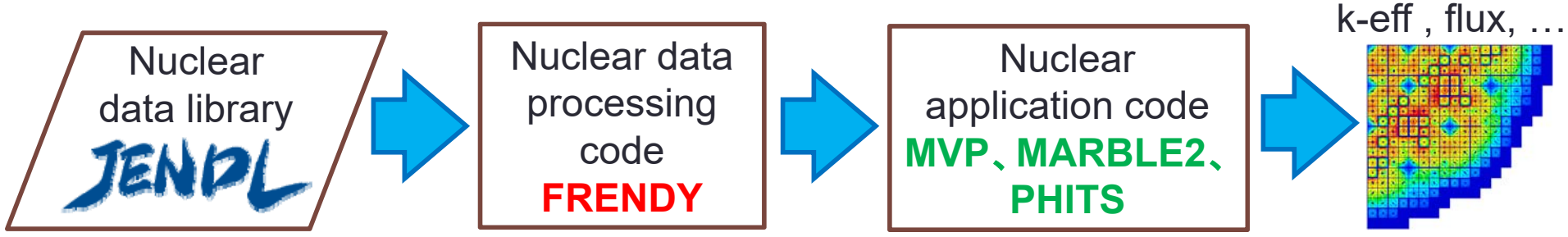


Present situation of nuclear data processing in JAEA

- 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



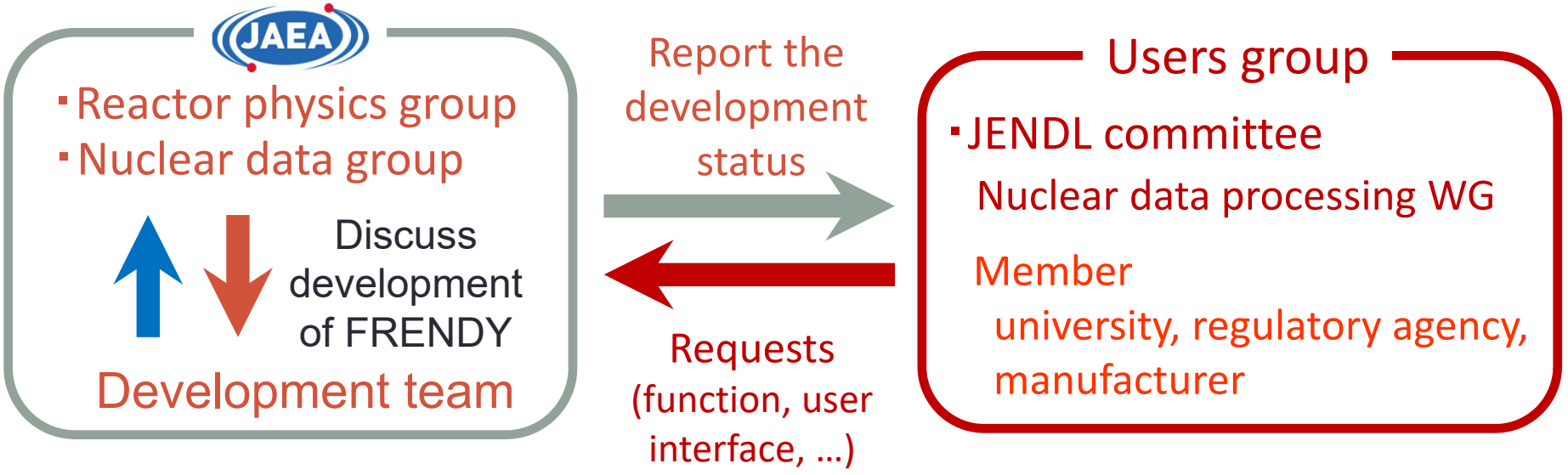
Features of FRENDY

- 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)

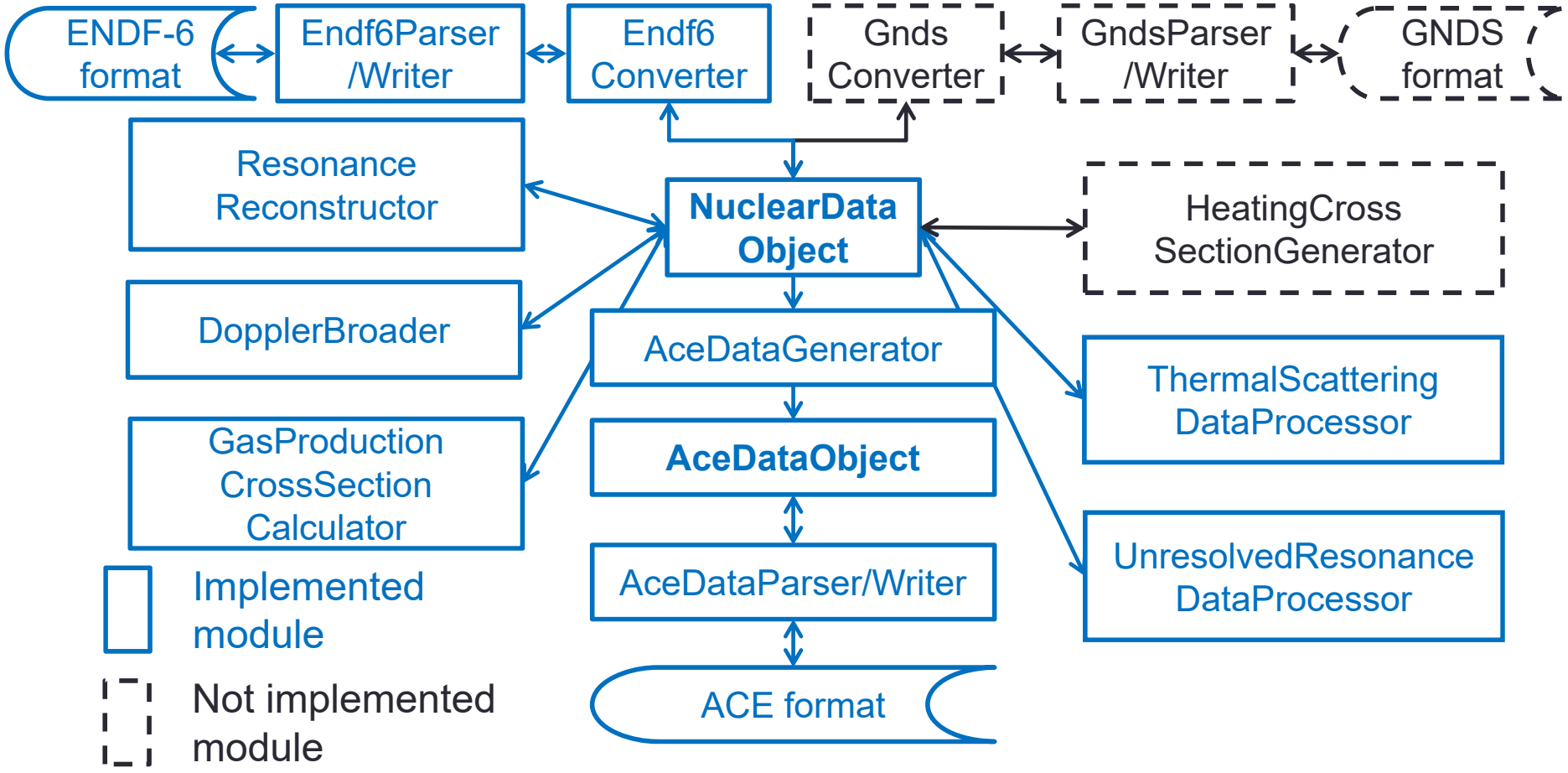
Development system of FRENDY

- 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/

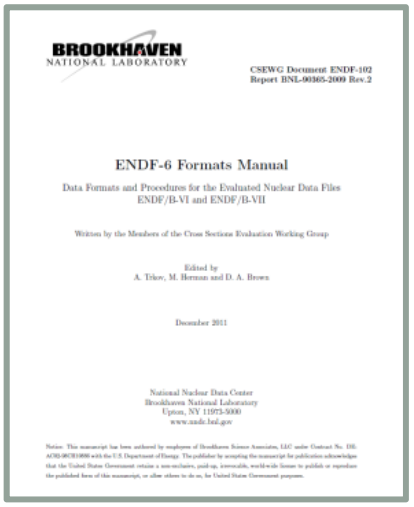
Example of ENDF-6 format (MF=3)

(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		099999	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
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[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="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>
```

Interpolation

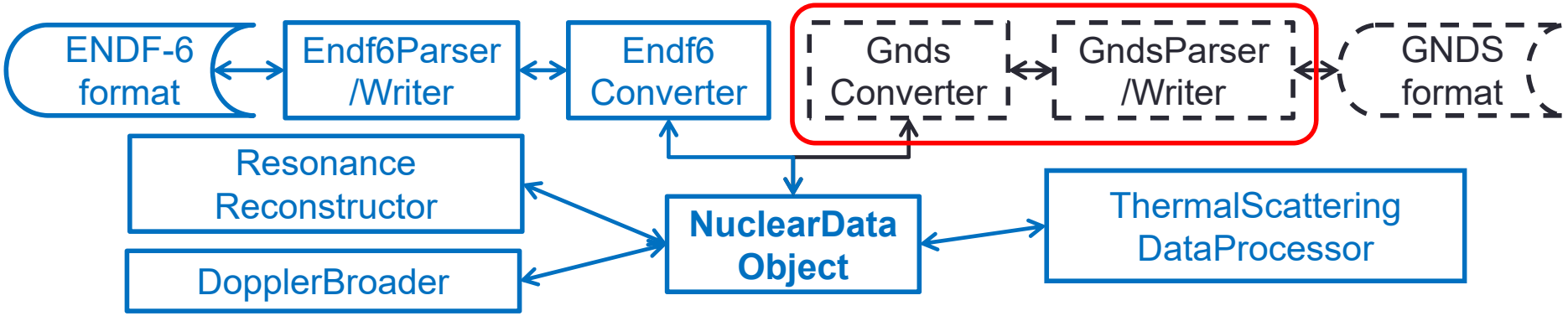
Cross section data

Secondary energy and angular distribution

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

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  5  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                            /
```

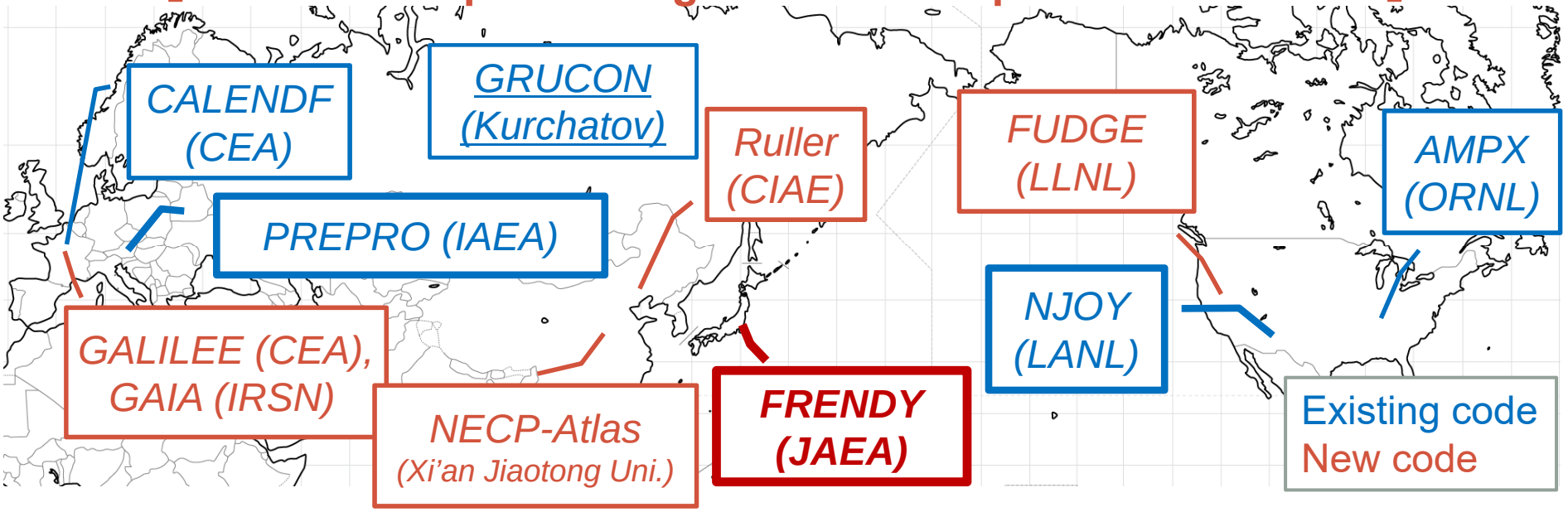
Development schedule of FRENDY

- 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

Collaboration with international organizations

- Participation of "ACE File Verification Project" proposed by IAEA
- Introduction of FRENDY to NDEC platform in OECD/NEA
  - After FRENDY is released

ACE File Verification Project

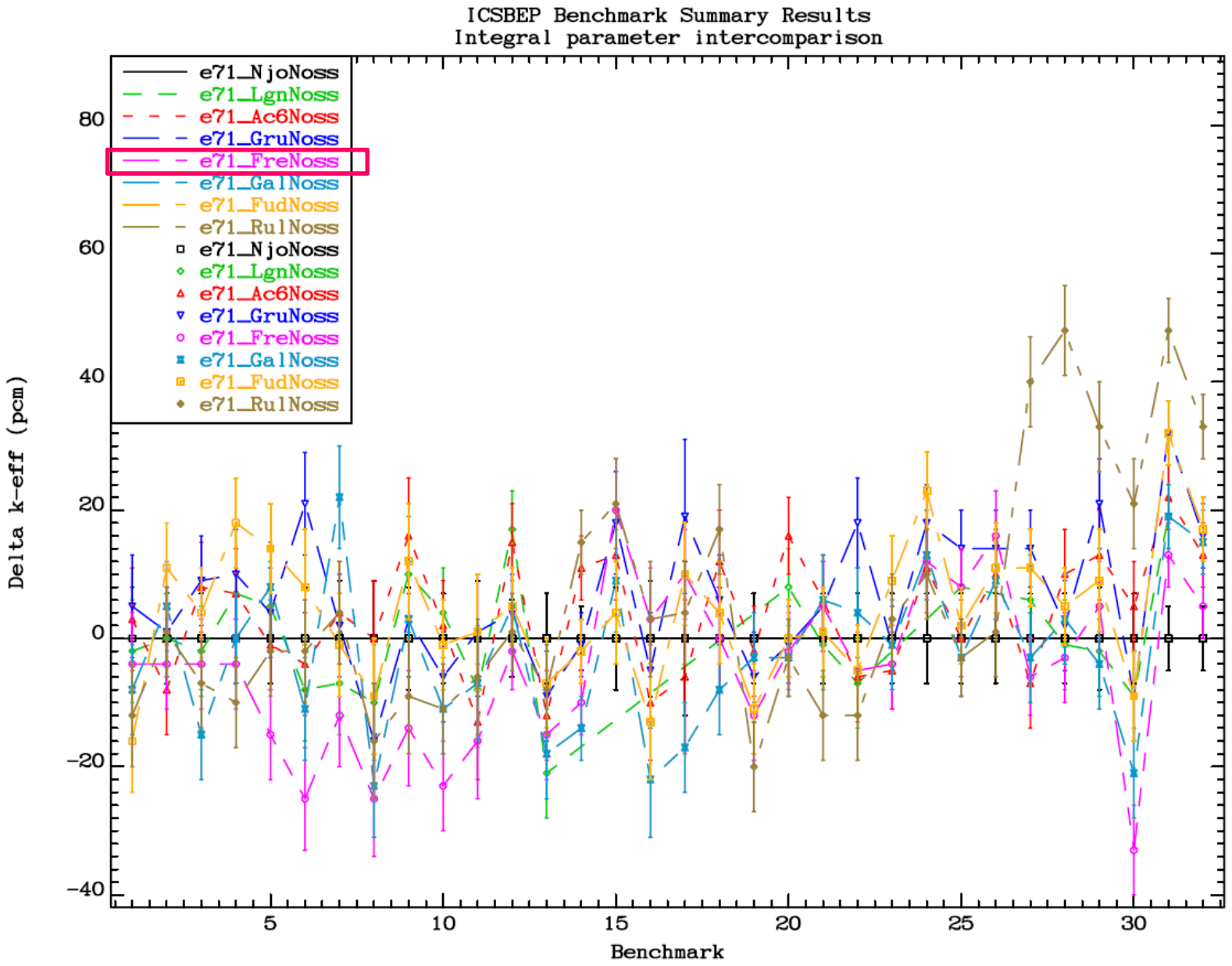
- Many nuclear data processing codes can generate ACE file
- IAEA proposed verification of nuclear data processing codes
  - ACE files of ^{235}U and ^{238}U from ENDF/B-VIII.β4 are compared
  - K-effective values of integral experiments analysis are also compared
- Participants : 9 institutes (10 codes)
  - **FRENDY(JAEA)**、NJOY2016、NJOY21(LANL)、FUDGE(LLNL)、PREPRO/ACEMAKER(IAEA/AENTA)、GRUCON(NRC)、Ruller(CIAE)、GAIA(IRSN)、Galilee(CEA)、NECP-Atlas(Xi'an Jiaotong University)

Project Stages of ACE File Verification Project

- Stage 1: ACE verification without self-shielding in URR
  - ACE files generated by nuclear data processing codes are similar to those by NJOY
  - Comparison results are reported on project web page
- Stage 2: ACE verification with self-shielding in URR
  - Now under going
  - Comparison results will be reported within a few months
- Stage 3: ACE verification of photon-production data
  - Comparison results will be reported at next summer
- Stage 4: ACE verification of thermal scattering (plan)

- ACE Verification Project
  - https://www-nds.iaea.org/ACE_verification/

Results of ACE Verification Project Stage 1



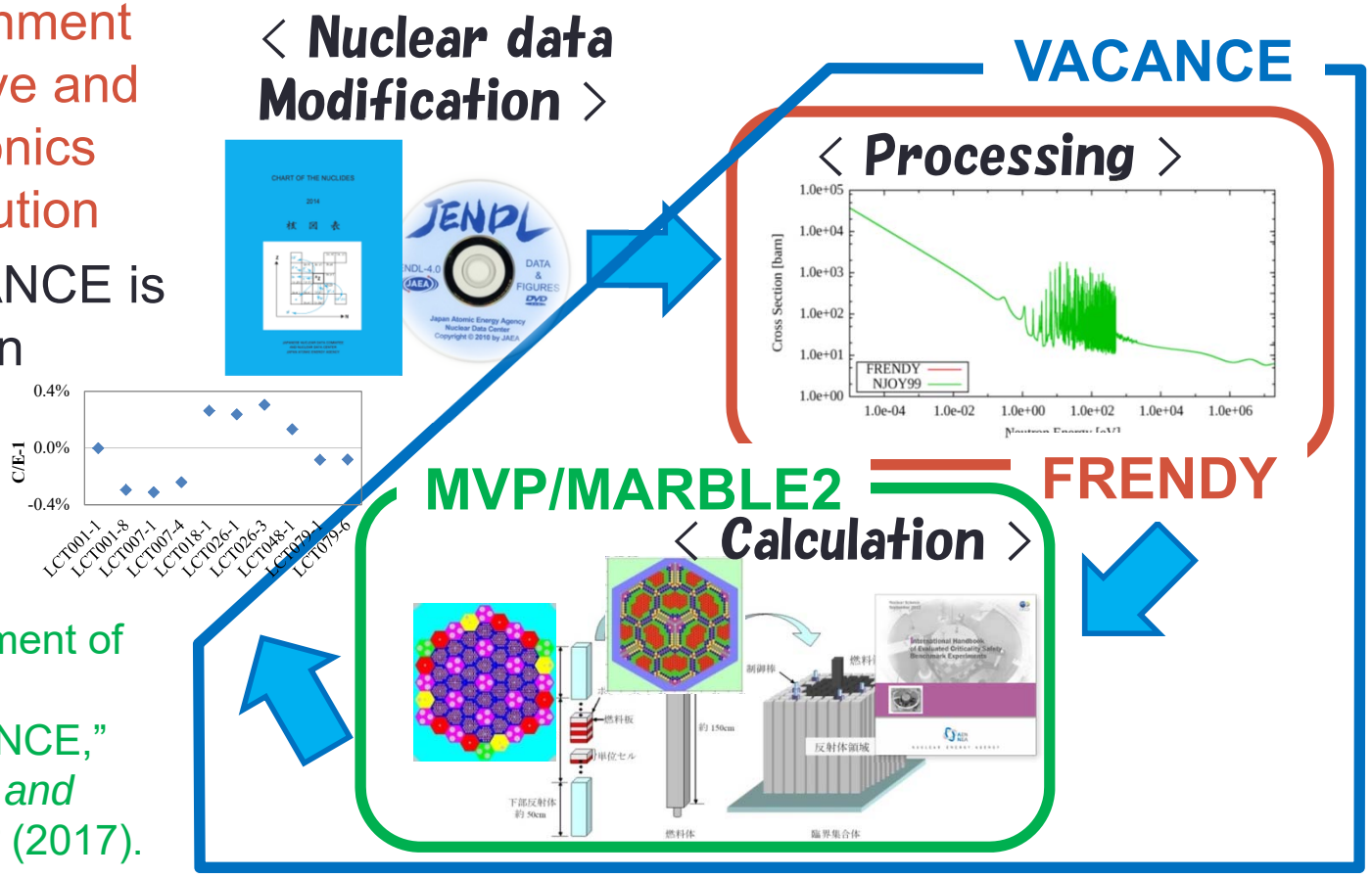
No.	Benchmark
1	hmf001
2	hmf002-002
3	hmf003-001
4	hmf003-002
5	hmf003-003
6	hmf003-010
7	hmf003-011
8	hmf014
9	hmf032-001
10	hmf032-002
11	hmf032-003
12	hmf032-004
13	icf004
14	imf007
15	imf007d
16	imf010
17	imf012
18	imf013
19	imf014-002
20	imf022-001
21	imf022-002
22	imf022-003
23	imf022-004
24	imf022-005
25	imf022-006
26	imf022-007
27	mif001-001
28	mif001-002
29	mif001-003
30	mif001-009
31	mif001-010
32	mif001-011

NDEC platform (OECD/NEA)

- OECD/NEA is developing NDEC platform for automatic verification, processing and verification of nuclear data
  - Current version of NDEC uses NJOY, PREPRO and FUDGE to generate ACE file
- OECD/NEA needs to include different processing codes
  - Diversifying production routes to generate ACE file
- NDEC
  - https://www.oecd-nea.org/dbdata/jeff/jeff33/NDEC_about.html

Validation of nuclear data in JAEA

- Development of automated nuclear validation system
- JAEA started developing an automatic nuclear data validation system **VACANCE** in 2016
  - **Va**lidation Environment for **C**omprehensive and **A**utomatic **N**eutronics **C**alculation **E**xecution
  - Concept of VACANCE is similar to NDEC in OECD/NEA



Ref.
K. Tada, et. al., Development of Automatic Nuclear Data Validation System VACANCE," *Proc. ICAPP2017, Fukui and Kyoto, Japan, Apr. 24-28* (2017).

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

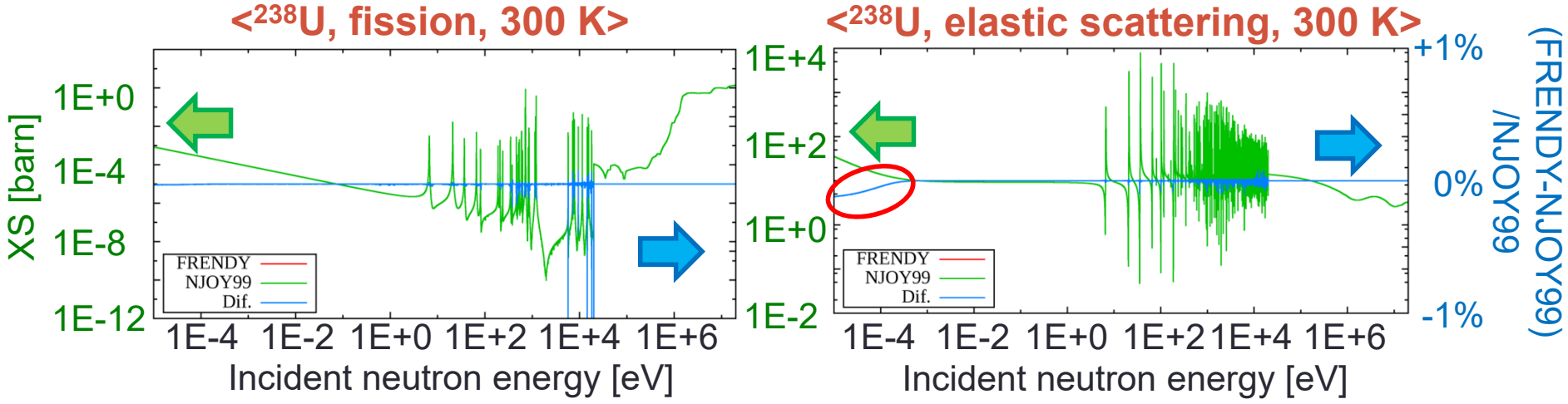
< Processing time [s] >

	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)

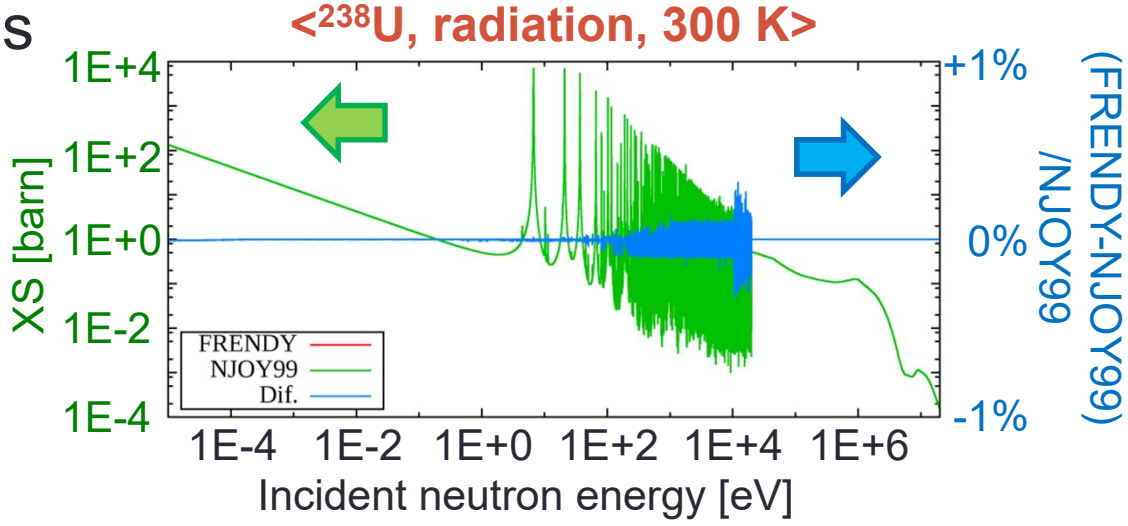
Comparison of Doppler broadening

- 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 1.0×10^{-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

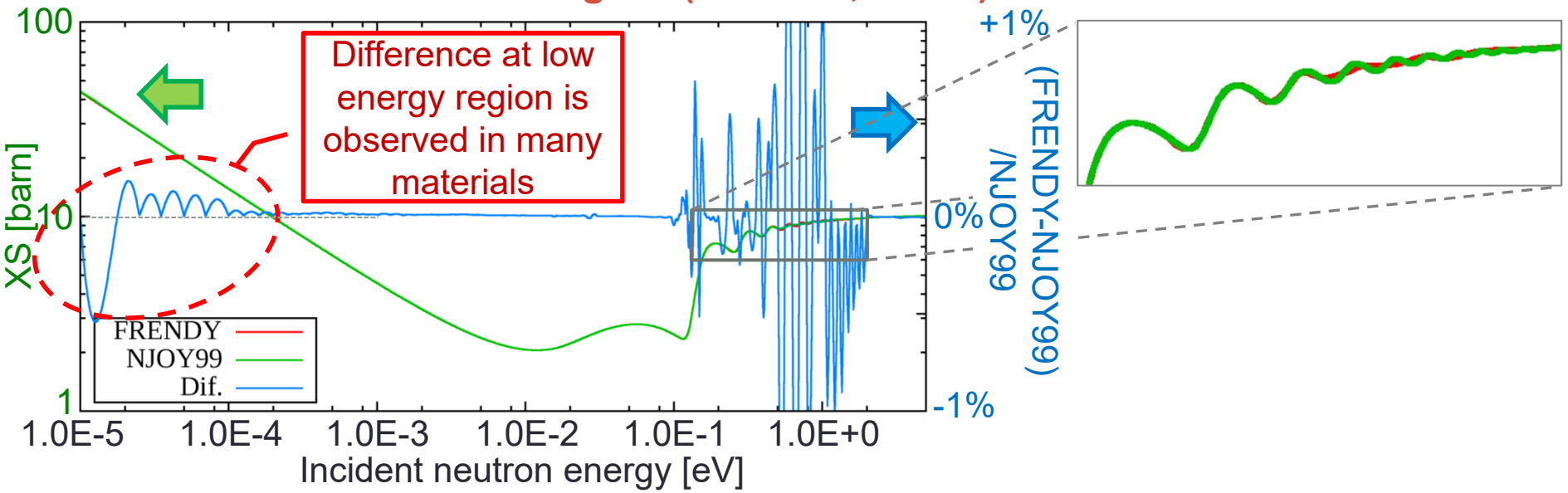
- The cross section at 0.0 eV is required to calculate the Doppler broadened cross section at low energy region
- NJOY approximates that the cross section follows the 1/v law
  - Since the elastic scattering cross section at the low energy region is constant, this approximation is not appropriate
- FRENDY 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 -

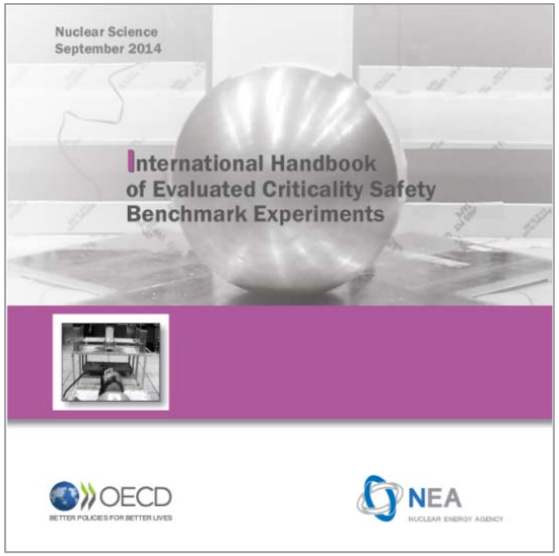
- NJOY only calculates the incoherent inelastic XS on 117 energy grids
  - Other energy grids are interpolated using the 5th order Lagrange interpolation
- The fixed energy grid is not appropriate for a material of which the cross section is oscillated
  - This difference may have impact on the TRIGA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

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



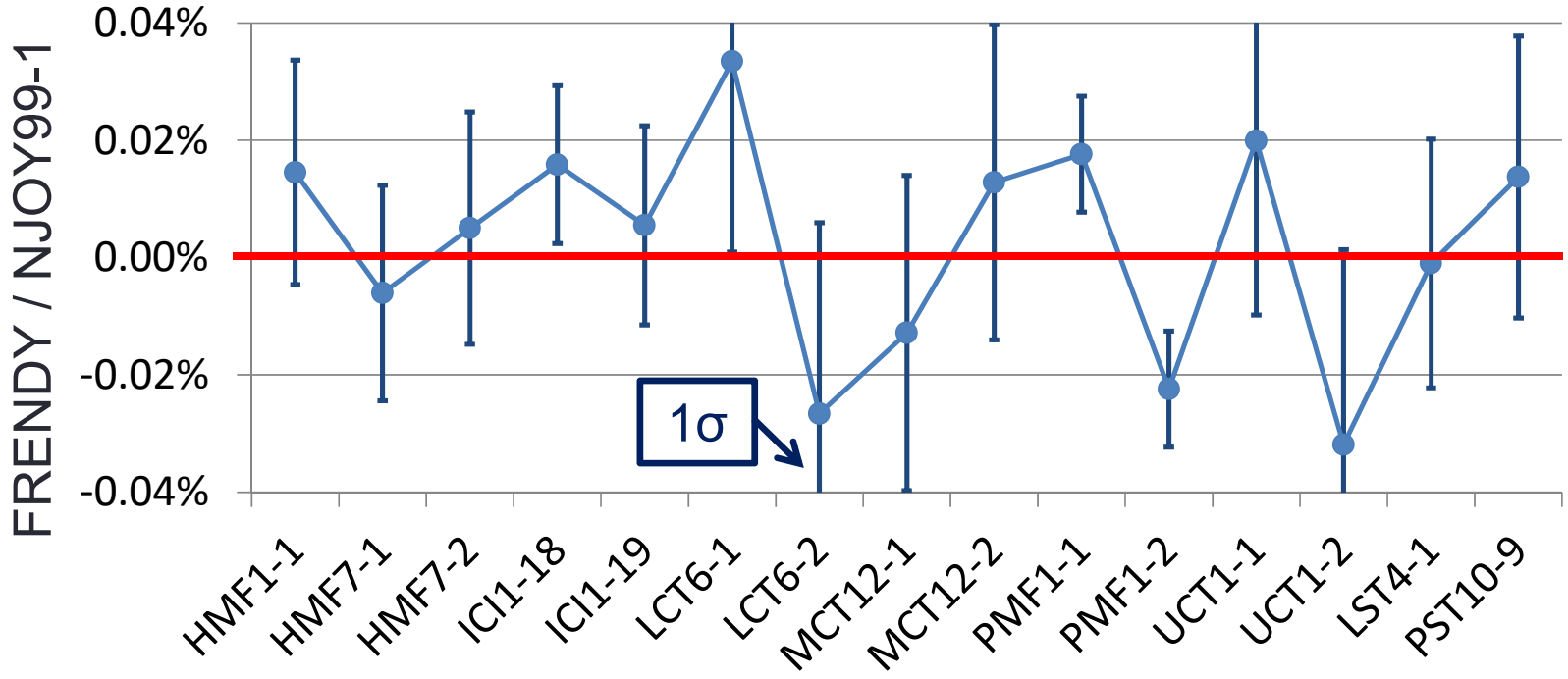
Verification of ACE file generating function

- 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