Ongoing developments for supporting Nuclear Data activities at NEA/DB

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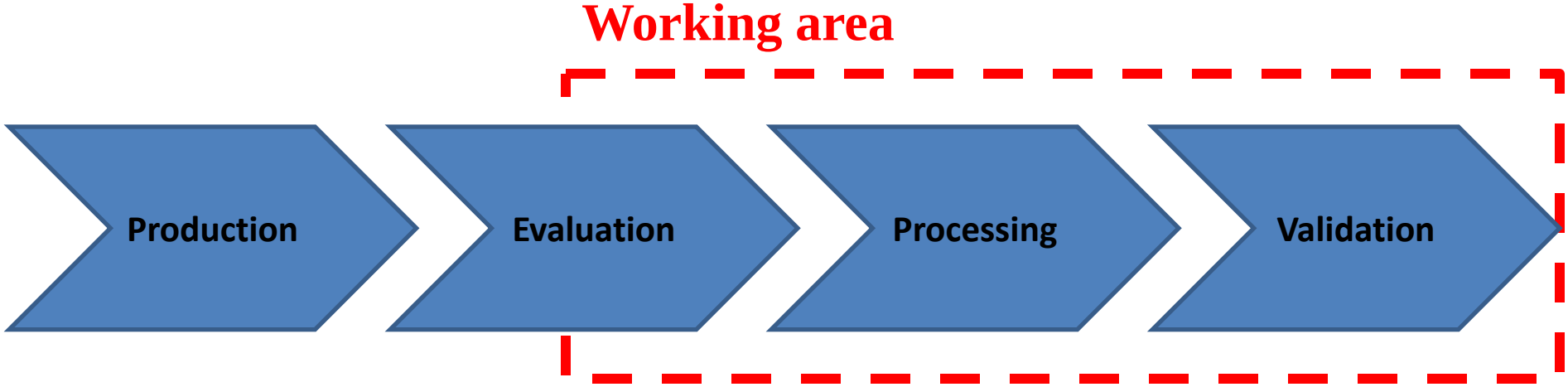
NEA Data Bank

In collaboration with James Dyrda, Ian Hill, Nicolas Soppera

1. Introduction

Our proposal for the Nuclear Data Evaluation Cycle (NDEC)

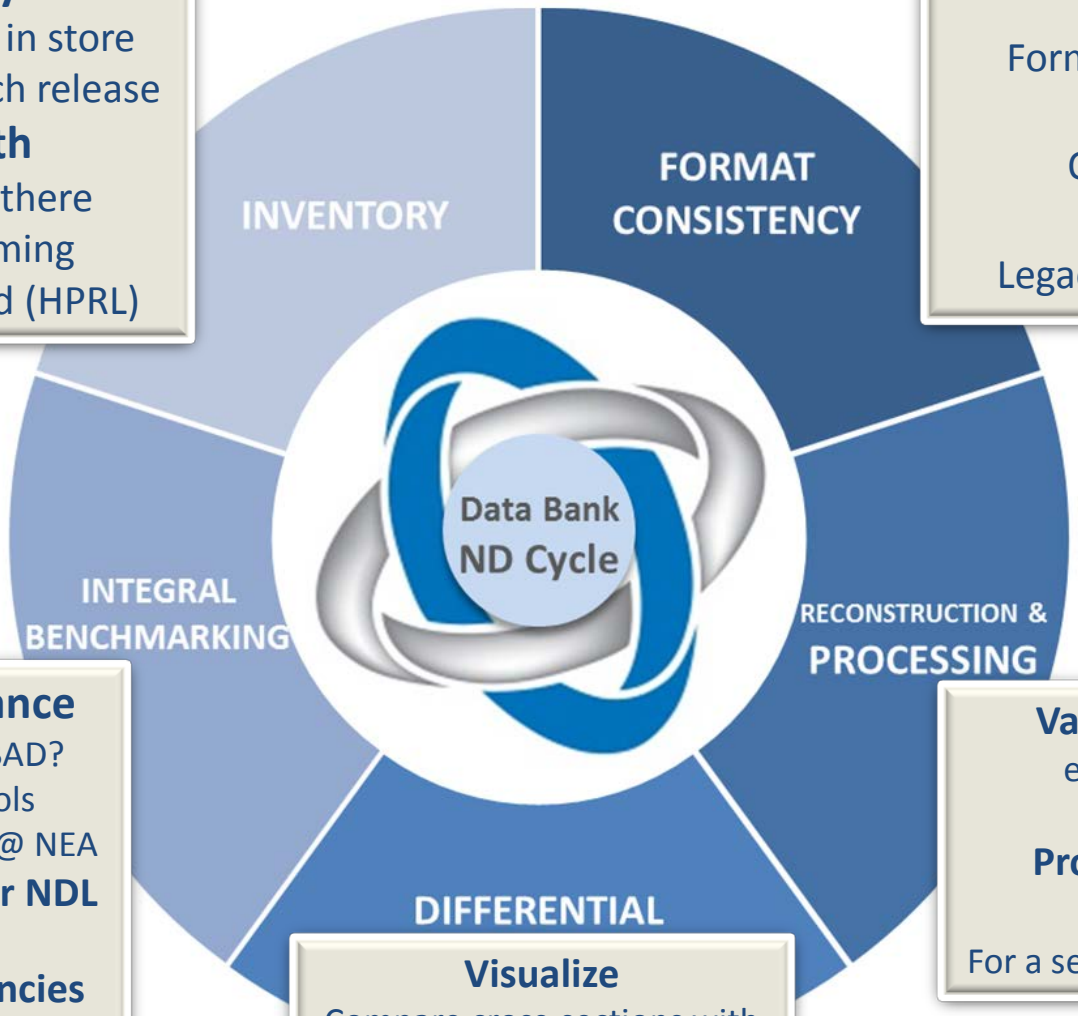


NEA/DB aims to

- Provide a tool/system/platform to facilitate the verification and validation of nuclear data: →**NDEC system**
- **Versioning system** for archiving nuclear data files (with their performance, and their evolution)

Identify
What we have in store
Who did it, which release
Link with
What is out there
What is coming
What is needed (HPRL)

Check
Format compliance
Interpret
Output Logs
Solve
Legacy errors in files



Assess Performance
ICSBEP, IRPHEP, SINBAD?
DICE sensitivity tools
4000+ cases available @ NEA
Compare with other NDL
ENDF, JENDL
Diagnose Discrepancies
Simplified numerical benchmarks ?

Validate Processing
e.g. NJOY, PREPRO, AMPX
Provide Application Libraries
For a selection of Temperatures

Visualize
Compare cross-sections with other NDL & EXFOR (JANIS)
Flag Discrepancies, Assess Library Quality
Statistical Metrics, Trending

2. Current status of developments

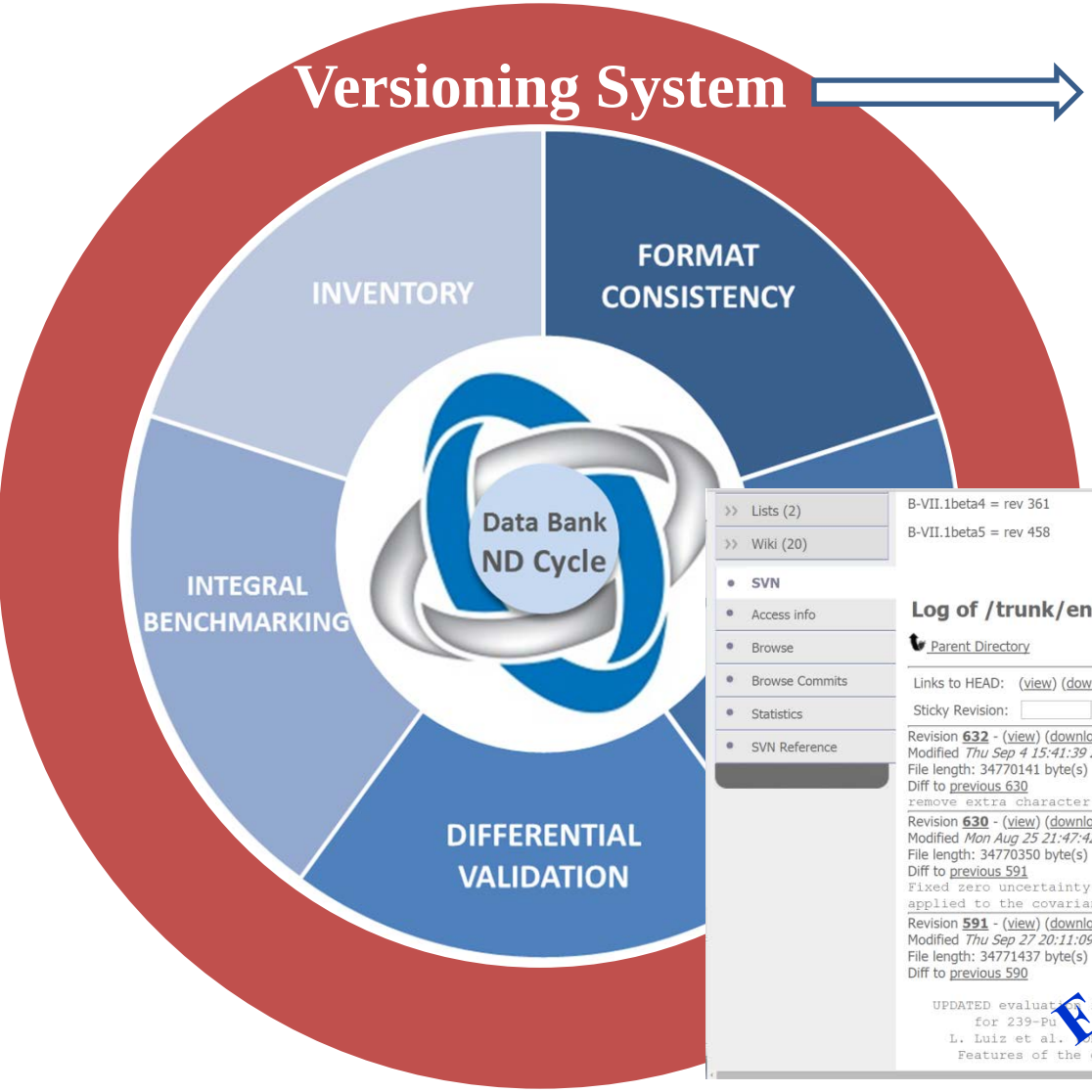
Current status: NDEC system

Objectives:

- Provide ND files with a minimum quality (checking, verification and validation)
- Help evaluators&end-users with understandable diagnose

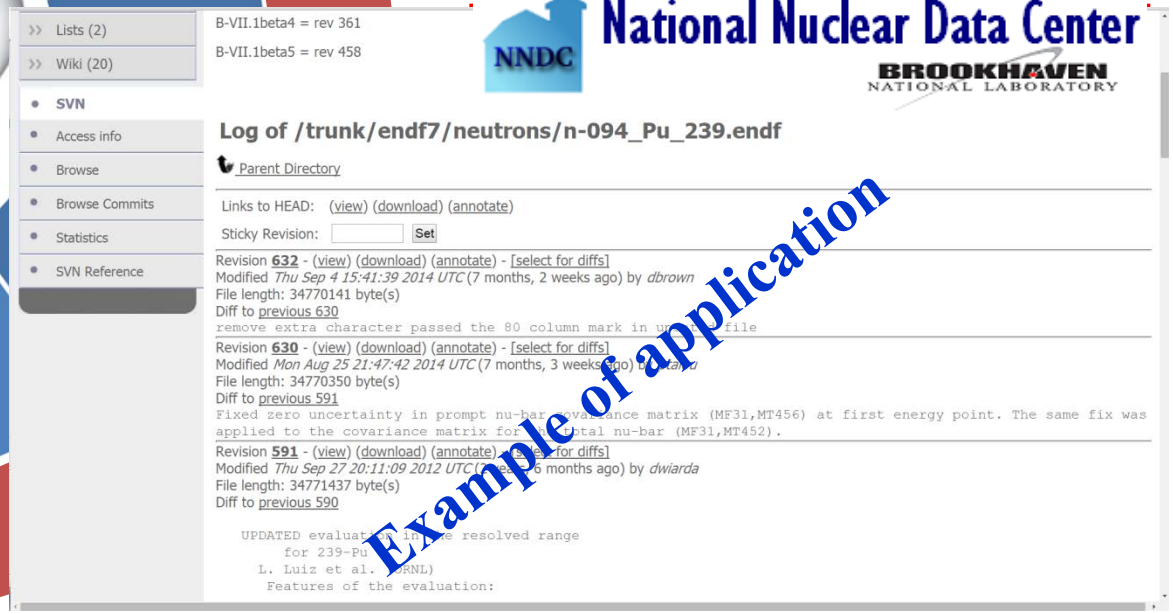
Finalising the PoC

Current status: Versioning System



Objectives:

- Archiving files for each version
- Keep track of bugs/modifications
- Implement easily accessible website for checking status of files



3. Application to Fe56

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Clickable tags for seeing content

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Main information of the file

nuclide	filename
26-Fe-56	fe56_cielo_v2.endf

Additional content to be added

MAT	Nuclide	File	Version	Last modification	New/Old evaluation	Comments	Evaluators	Institution	Reference
2625	Fe-56	n-26-Fe-056.jeff33	rev33.0	01/12/2017	Mix updates: rev32.1 + rev32.4	Inclusion of new EXFOR data	A. BCD, E. FGH, I. JKL	XXX	CHANDA-DXXX

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Processing Fe56 CIELO v2 ENDF-6 file

https://www-nds.iaea.org/CIELO/data/fe56v02_endf.zip

Summary report of processing codes

ENDF Check and Utilities Codes			
stanef	checkr	fizcon	psyche
Warnings: 0	Warnings: 1	Warnings: 1	Warnings: 0
Errors: 0	Errors: 0	Errors: 0	Errors: 0

PRERPRO 2012				
LINEAR	RECENT	SIGMA1	FIXUP	DICTIN
Warnings: 0	Warnings: 0	Warnings: 0	Warnings: 0	Warnings: 0
Errors: 0	Errors: 0	Errors: 0	Errors: 0	Errors: 0

NJOY2012									
moder	reconr	broadr	heatr	gaspr	thermr	purr	acer-maker	acer-checker	groupr
Warnings: 0	Warnings: 0	Warnings: 0	Warnings: 0	Warnings: 0	Warnings: 0	Warnings: 1	Warnings: 10	Warnings: 27	Warnings: 5
Errors: 0	Errors: 0	Errors: 0	Errors: 1	Errors: 1	Errors: 0	Errors: 0	Errors: 0	Errors: 0	Errors: 0

- **ENDF C&U codes, PREPRO12/15, NJOY2012 run automatically**
- **AMPX run manually**

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Errors: 0	Errors: 0	Errors: 0	Errors: 1	Errors: 1	Errors: 0	Errors: 0	Errors: 0	Errors: 0	Errors: 0

- Modules run displayed
- Colour scheme depending on warning/error messages
- Warning/error counter

3. Application to Fe56

NDEC System/Platform

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Errors: 0	Errors: 0	Errors: 0	Errors: 1	Errors: 1	Errors: 0	Errors: 0	Errors: 0	Errors: 0	Errors: 0

Module: acer-maker

Files:

- Output:
- Messages: acer-maker.msg

For each module

Summary view
Access to inputs/outputs

Amount	Warning/Error type	Message	Description
9	acer2	---message from ptleg2---negative probs found	This message indicates that a negative PDF value was found; NJOY sets the value to zero and renormalizes the distribution
1	acer4	---message from unionx---threshold error	This message normally surfaces when there is an inconsistency between the threshold energy of a reaction in the ENDF file and the value calculated by NJOY. This is already checked and corrected in reconr so this message should never occur again. However, NJOY uses ENDF files to transfer information between modules in which any number is rounded to 6 significant digits. In the case of the above mentioned nuclides, the difference between the calculated value and the one in the ENDF file occurs in the 7th significant digit (which is lost due to rounding).

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Processing Fe56 CIELO v2 ENDF-6 file

Summary report of processing codes

NJOY2012									
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Warnings: 0	Warnings: 0	Warnings: 0	Warnings: 0	Warnings: 0	Warnings: 0	Warnings: 1	Warnings: 10	Warnings: 27	Warnings: 5
Errors: 0	Errors: 0	Errors: 0	Errors: 1	Errors: 1	Errors: 0	Errors: 0	Errors: 0	Errors: 0	Errors: 0

Module: acer-maker

Files:

- Output:
- Messages: acer-maker.msg

Human readable description +hints of problem's source

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Warning/Error classification

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Processing Fe56 CIELO v2 ENDF-6 file

Summary report of Differential Validation

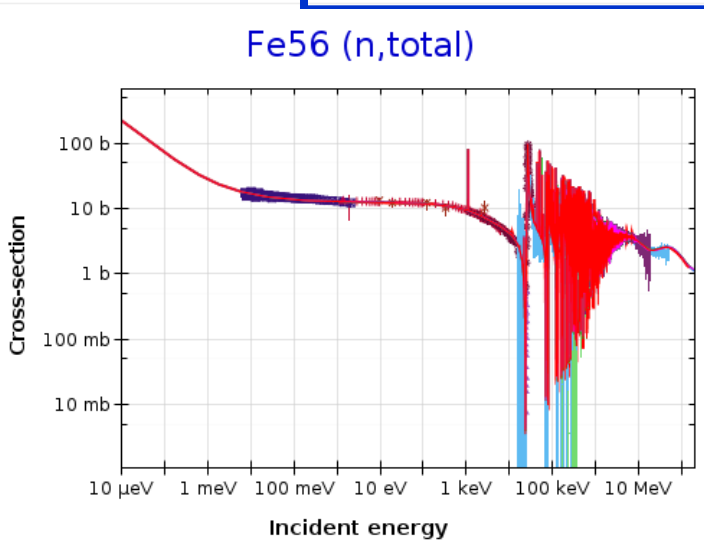
ABSOLUTE PLOTS	COMPARISON PLOTS	INTER

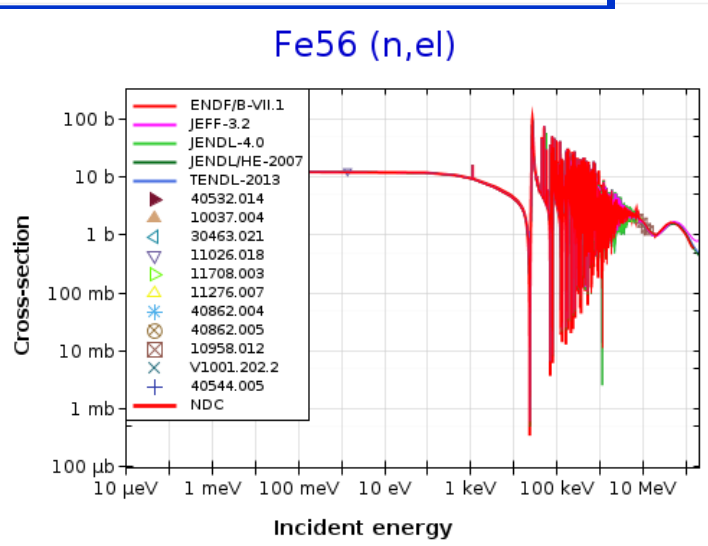
Cross section comparison with main nuclear data libs + EXFOR

Fe-56 CIELO v2 file

- **ABSOLUTE PLOTS**

- Cross section MT 1
- Cross section MT 2
- Cross section MT 4
- Cross section MT 5
- Cross section MT 16
- Cross section MT 22
- Cross section MT 28
- Cross section MT 51
- Cross section MT 52
- Cross section MT 53
- Cross section MT 54
- Cross section MT 55
- Cross section MT 56
- Cross section MT 57





3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Processing Fe56 CIELO v2 ENDF-6 file

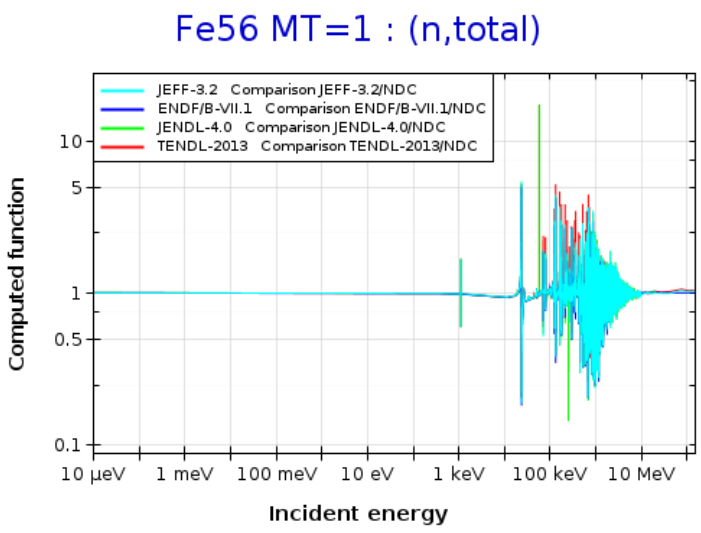
Summary report of Differential Validation

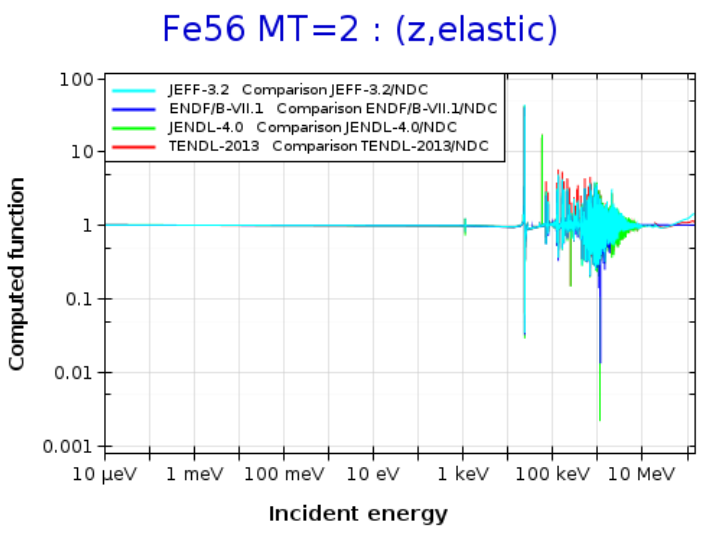
ABSOLUTE PLOTS	COMPARISON PLOTS	INTER

Processed lib compared against main ones

Fe-56 CIELO v2 file

- **COMPARISON PLOTS**
- Cross section MT 1
- Cross section MT 2
- Cross section MT 4
- Cross section MT 16
- Cross section MT 22
- Cross section MT 28
- Cross section MT 51
- Cross section MT 52
- Cross section MT 53
- Cross section MT 54
- Cross section MT 55
- Cross section MT 56
- Cross section MT 57
- Cross section MT 58





3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Processing Fe56 CIELO v2 ENDF-6 file

Summary report of Differential Validation

ABSOLUTE PLOTS	COMPARISON PLOTS	INTER

Fe-56 CIELO v2 file

- **COMPARISON PLOTS**

- Cross section MT 1
- Cross section MT 2
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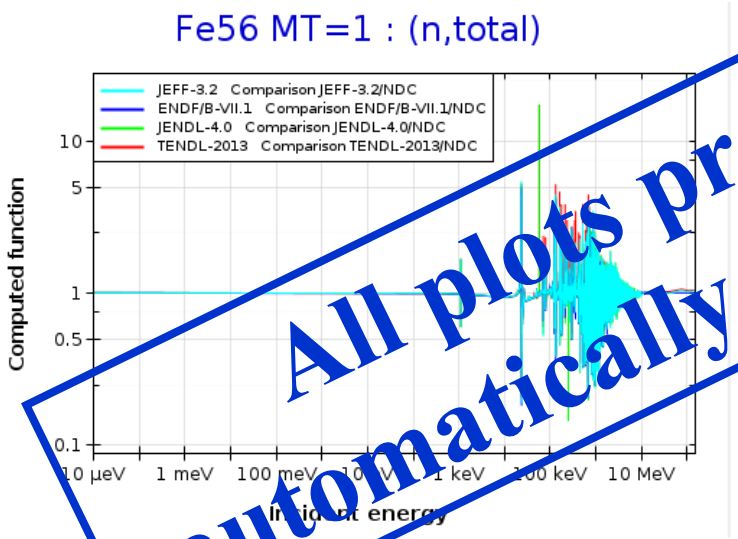
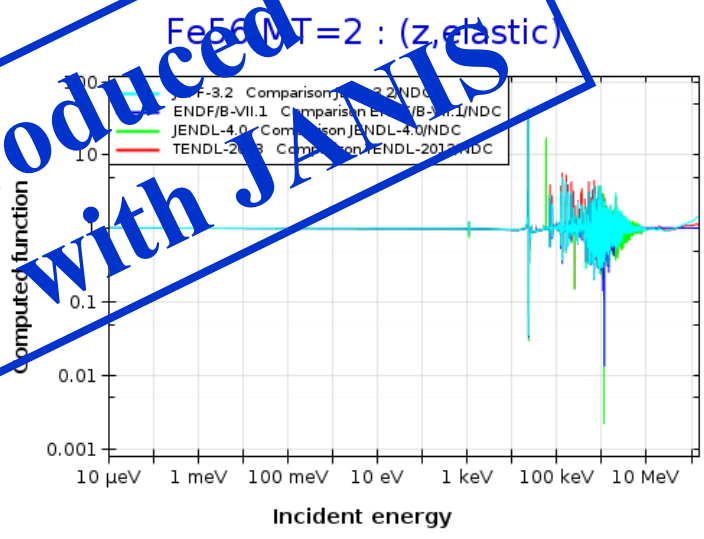




All plots produced automatically with JANIS

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Processing Fe56 CIELO v2 ENDF-6 file

Objective: Seeing the performance of the processed file (with different libraries as basis)

Automatized integral validation not yet implemented

However,

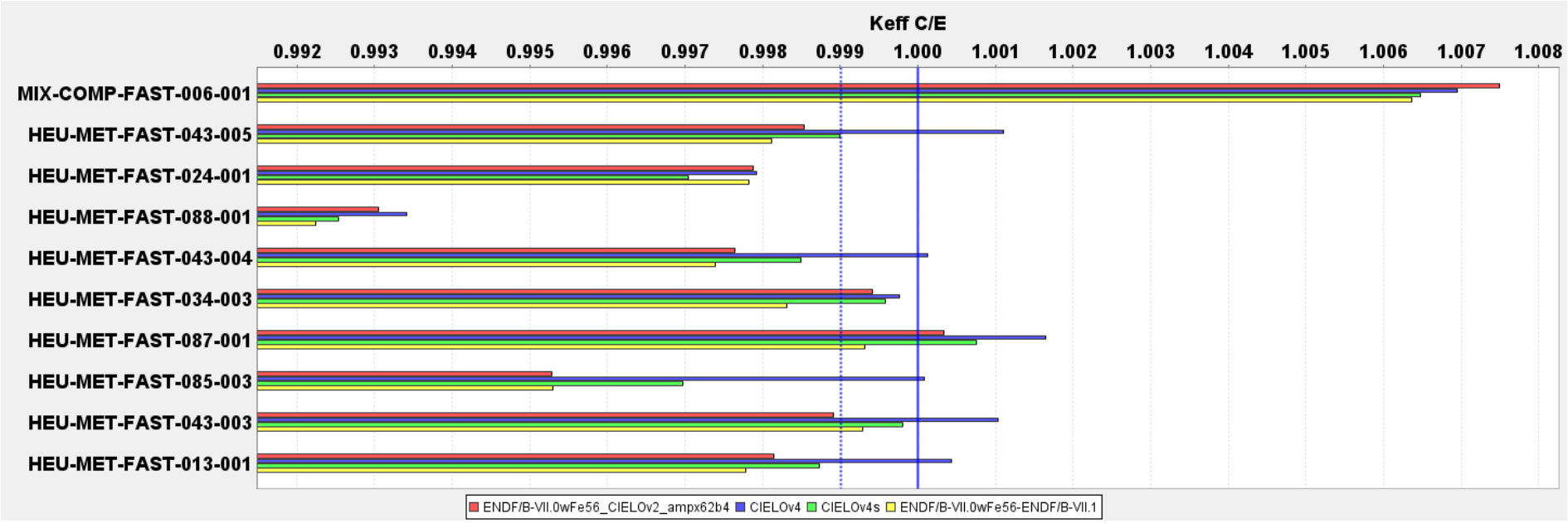
- Selection of most relevant benchmarks with DICE database (ICSBEP), based of sensitivity analysis + expertise.
- **Selected benchmarks run with SCALE**.
- Comparison plots generated with DICE.

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Processing Fe56 CIELO v2, v4 and v4s ENDF-6 file



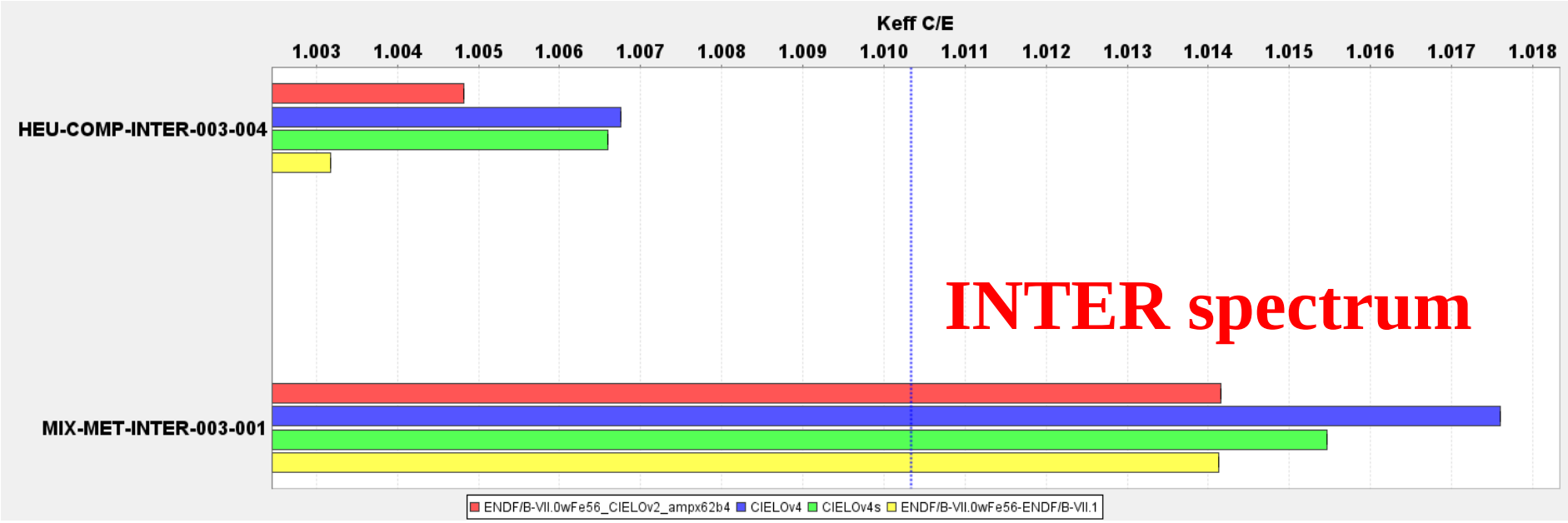
CIELOv2, CIELOv4, CIELOv4s, ENDF/B-VII.1

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Processing Fe56 CIELO v2, v4 and v4s ENDF-6 file



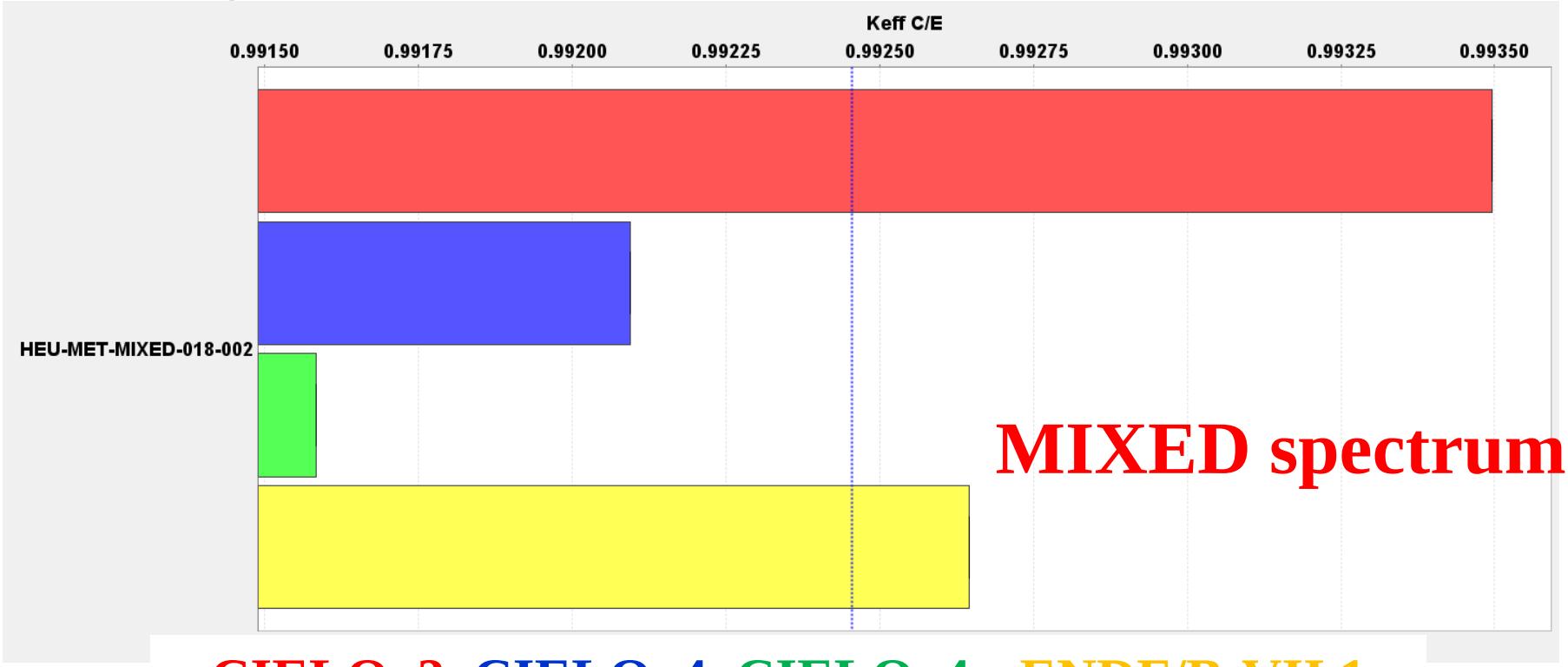
CIELOv2, CIELOv4, CIELOv4s, ENDF/B-VII.1

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Processing Fe56 CIELO v2, v4 and v4s ENDF-6 file



MIXED spectrum

CIELOv2, CIELOv4, CIELOv4s, ENDF/B-VII.1

3. Application to Fe56

NDEC System/Platform

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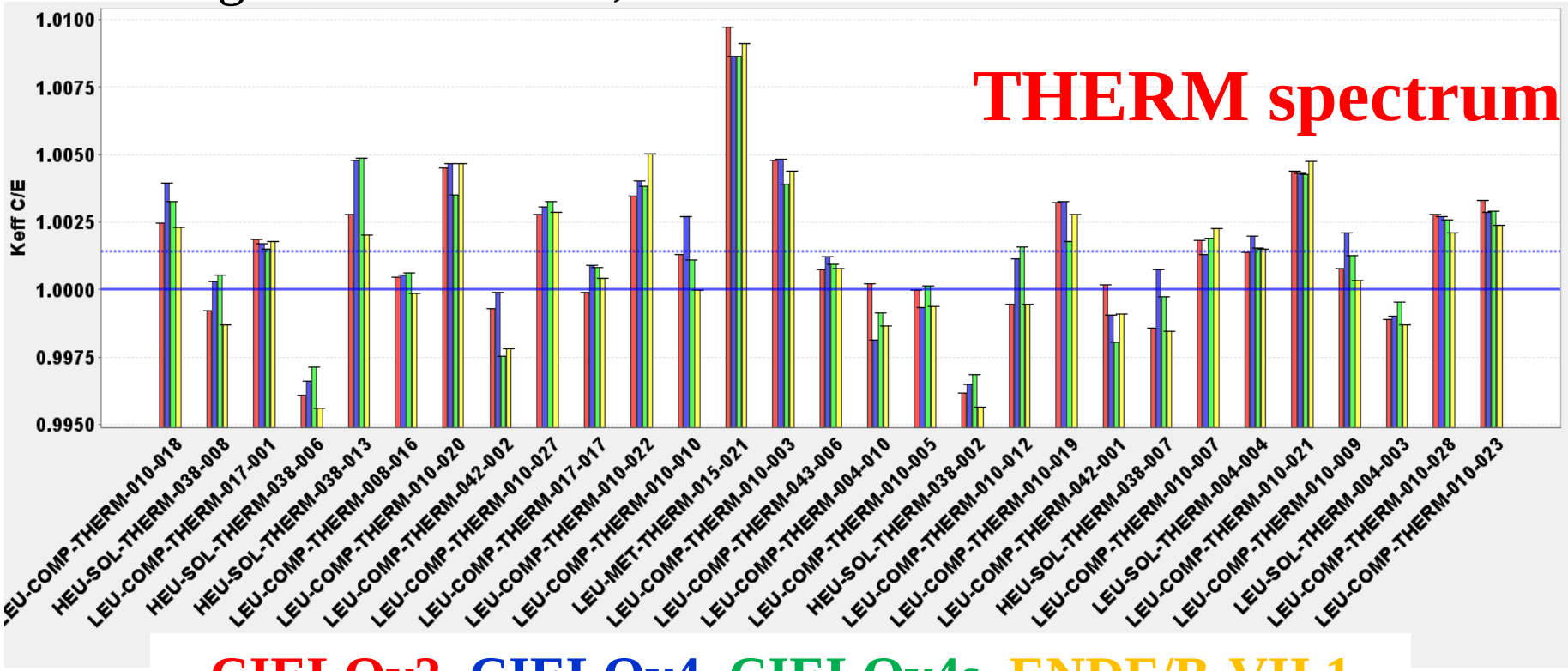
Processing Fe56 CIELO v2, v4 and v4s ENDF-6 file



CIELOv2, CIELOv4, CIELOv4s, ENDF/B-VII.1

3. Application to Fe56

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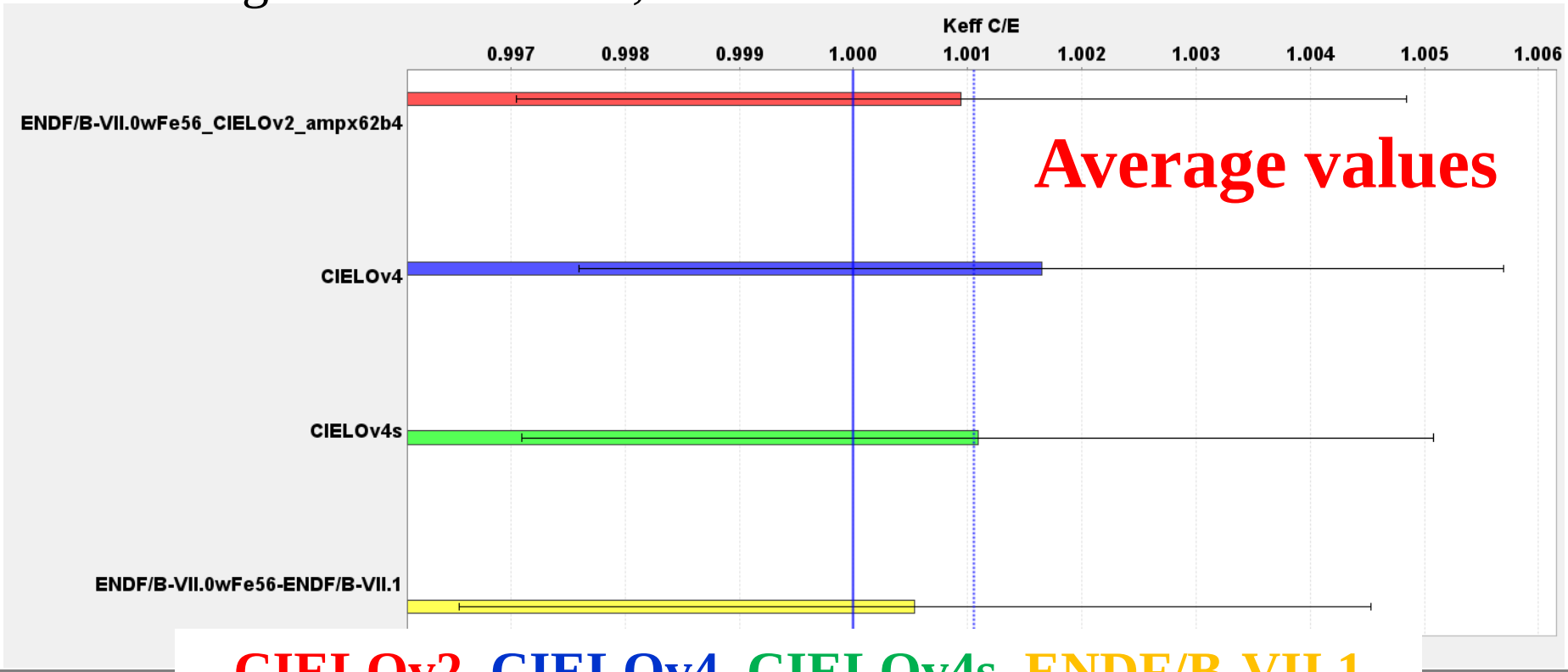

CIELOv2, CIELOv4, CIELOv4s, ENDF/B-VII.1

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Processing Fe56 CIELO v2 ENDF-6 file

	ENDF/B-VII file		CIELOv2 file		Difference(pcm) CIELOvsENDF/B
HEU-COMP-INTER-003-004	1.00317	0.00029	1.00482	0.00029	164
HEU-MET-FAST-034-003	0.99731	0.00028	0.99842	0.00029	111
HEU-MET-FAST-087-001	0.99802	0.00029	0.99904	0.00029	102
IEU-MET-FAST-005-001	1.00214	0.00029	1.00106	0.00029	-108
LEU-COMP-THERM-004-010	0.99844	0.00061	1.00001	0.00088	157
LEU-COMP-THERM-010-010	0.99999	0.00045	1.0013	0.00055	131
LEU-COMP-THERM-010-022	1.00503	0.00049	1.00346	0.00053	-156
LEU-COMP-THERM-010-023	1.00237	0.00049	1.00329	0.00046	92
LEU-COMP-THERM-042-001	0.9991	0.0011	1.00016	0.00084	106
LEU-COMP-THERM-042-002	0.9978	0.001	0.9993	0.001	150
MIX-COMP-FAST-006-001	0.9952	0.00016	0.99631	0.00017	112

Largest difference ~160pcm

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Explaining large differences between ENDF/B-VII and JEFF-3.2

- Sensitivity Analysis provides positive bias ~ + 150pcm
- Swapping MF4 MT2 produces (Direct calculation) ~ - 329 pcm

	ENDF/B-VII file		CIELOv2 file		Difference(pcm) CIELOvsENDF/B	JEFF-3.2 file		Difference(pcm) JEFFvsENDF/B
PU-MET-FAST-028-001	0.99783	0.00029	0.99696	0.0003	-87	0.99445	0.00035	-339
MIX-COMP-FAST-006-001	0.9952	0.00016	0.99631	0.00017	112	0.99679	0.00017	160

Importance of angular distribution data (and their sensitivities)

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Explaining large differences between ENDF/B-VII and JEFF-3.2

- Sensitivity Analysis provides positive bias (~+160pcm)
- Differences between direct calculations produces same result

	ENDF/B-VII file		CIELOv2 file		Difference(pcm) CIELOvsENDF/B	JEFF-3.2 file		Difference(pcm) JEFFvsENDF/B
PU-MET-FAST-028-001	0.99783	0.00029	0.99696	0.0003	-87	0.99445	0.00035	-339
MIX-COMP-FAST-006-001	0.9952	0.00016	0.99631	0.00017	112	0.99679	0.00017	160

However, impact of angular distribution data have to be checked

3. Application to Fe56

NDEC System/Platform

FILE INFORMATION	PROCESSING REPORT	DIFFERENTIAL TESTING	INTEGRAL TESTING

Explaining large differences between ENDF/B-VII and JEFF-3.2

Work to be acknowledged to
Ian Hill and James Dyrda (NEA)

4. Conclusions & Future implementations

Conclusions

- Current PoC of NDEC almost fully finished
  → Start production stage?
- Automatized main processing codes
- Automatized plots generation with JANIS
- Easy visualization & interaction with results through a HTML page

General future implementations

- Integrate all scripts/process in a same code developing platform (likely JAVA, as done for JANIS and DICE)
- Automatize AMPX processing
- Automatize Integral validation with SCALE+MCNP
- Provide service online (soon?)
- Implement PoC versioning system

Detailed future implementations

- Info file:
  - Fill content by processing file or reviewing content

- Processing:
  - Links to inputs/outputs
  - Links to warning/error messages in outputs
  - Parser AMPX output for warning/errors
  - Improve warning/error dictionary
  - Parser thoroughly ENDF C&U outputs
  - Add FUDGE code to the list
  - Implement consistency checks: discontinuities, checkers for zero values non-expected, positive definite
  - Automatized main processing codes
  - Add processing for COG code ?

Detailed future implementations

- Differential testing:
  - Implementation of metrics for closeness to EXFOR data
  - Integrate JANIS completely in order to interact with the plots
  - Generation of GENDF data, and comparison between major libraries
  - Implementation of INTER for comparison of integrated cross section values

- Integral testing
  - Automatize search of most relevant benchmark (integrate DICE in NDEC)
  - Generation of expecting changes in benchmark based on sensitivity analysis (integrate NDaST in NDEC)
  - Automatize running of MCNP inputs and results retrieval
  - Automatize running of COG inputs and results retrieval ??

We are looking forward to any feedback/collaboration!!

Thank you for your attention!!
Merci pour votre attention!!
Gracias por su atención!!

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