A new V&V philosophy for fusion nuclear data libraries

D. Laghi[1,2], M. Fabbri[3]
[1]NIER Ingegneria, Castel Maggiore, Italy
[2]University of Bologna, Bologna, Italy
[3]Fusion For Energy, Barcelona, Spain

11/10/2022

Jade

Powered By:

NIER

MAKING CHANGE HAPPEN. MAKING LIFE SMARTER.

ALMA MATER STUDIORUM A.D. 1088 UNIVERSITÀ DI BOLOGNA

DIPARTIMENTO DI INGEGNERIA INDUSTRIALE

FUSION FOR ENERGY

Index

JADE

- Nuclear data libraries and their V&V
- What is JADE?
- The Sphere Leakage benchmark
- JADE architecture and development

Looking ahead

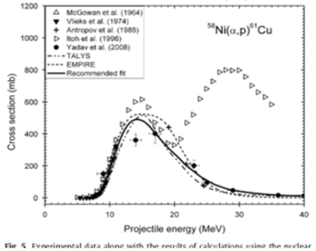
- Our wish list
- Machine Learning
- Summary

JADE

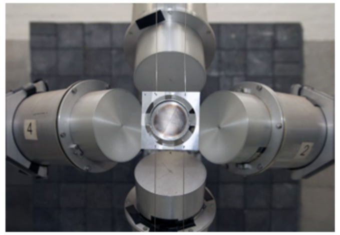
Nuclear data libraries and their V&V

The nuclear data libraries production chain

Theoretical support



Experimental points



Analytical models

Nuclear data processing code [NJOY]

Evaluated continuous cross sections

[ENDF 6 format]

Point-wise/multi-group cross sections

[ACE format]

MC Transport codes MCNP6

It is a complex procedure that require extensive Verification and Validation (V&V)

Nuclear data libraries and their V&V

The need for automation and standardization

10^3 isotopes in a single library

1 .ACE file per isotope

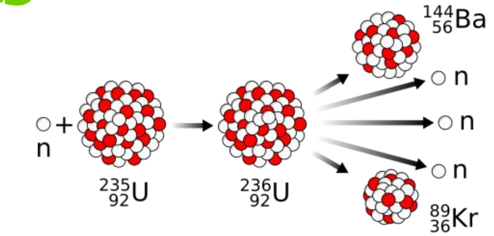
10^2 reactions per .ACE file (MT numbers)

~ 10^5 different cross sections to be verified!

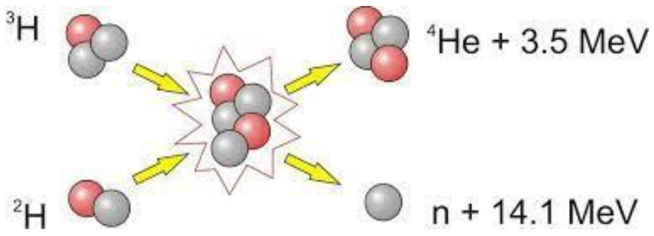
Heavy automation is a necessity, which, at the same time, is an opportunity for standardization

Nuclear data libraries and their V&V

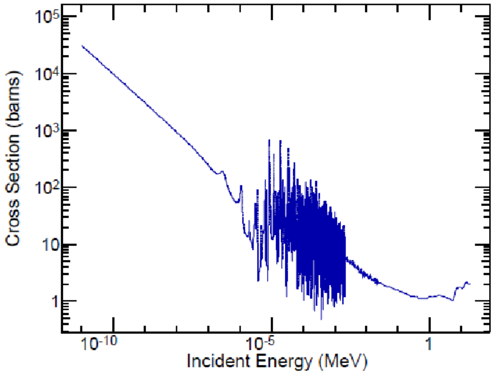
The fission bias

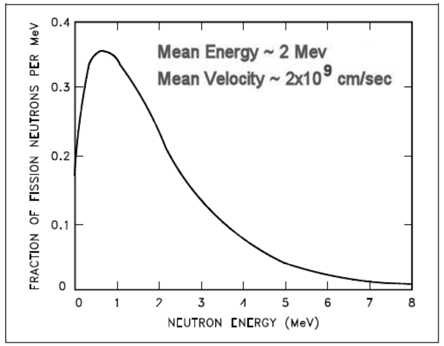


Vs

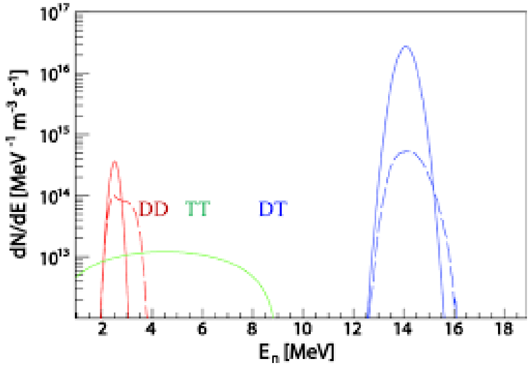


Energy range





Prompt Fission Neutron Energy Spectrum for Thermal Fission of Uranium-235

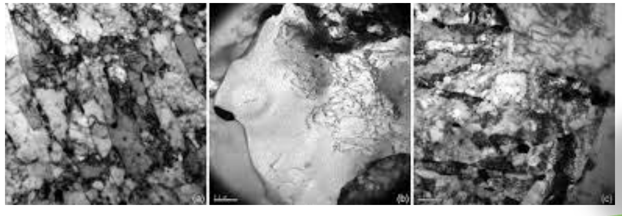


Different materials and cross sections

Fission rate

Fission products

EUROFER 97



Fusion rate

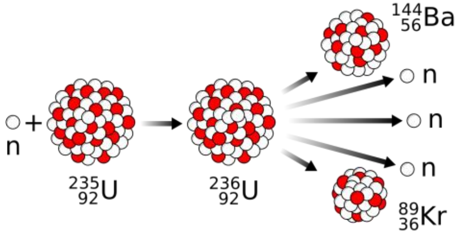
Tritium production

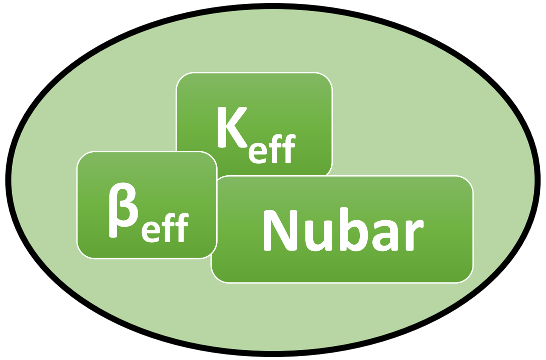
Activation issues

Heating on superconductive magnets

Nuclear data libraries and their V&V

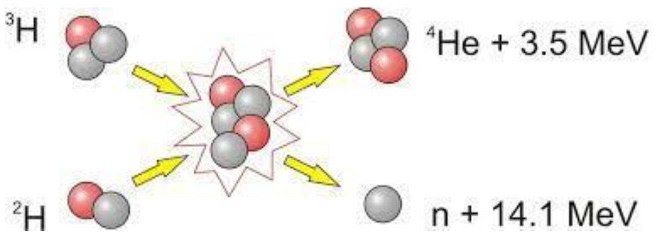
The fission bias

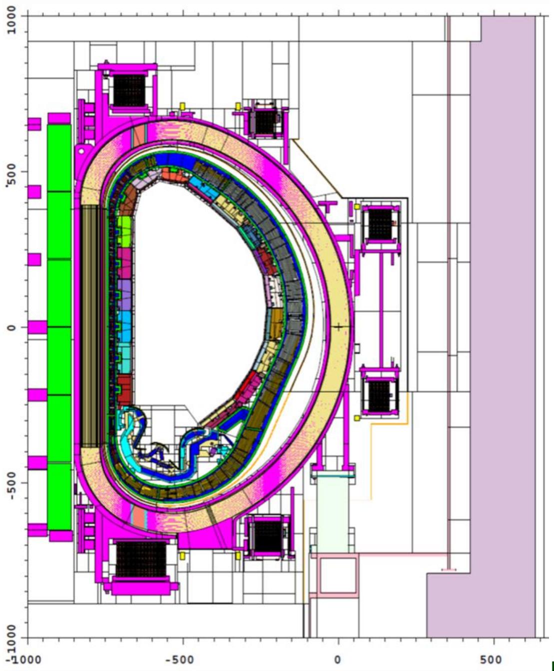




Integral parameters representative of the entire system that simplifies the V&V process

Vs





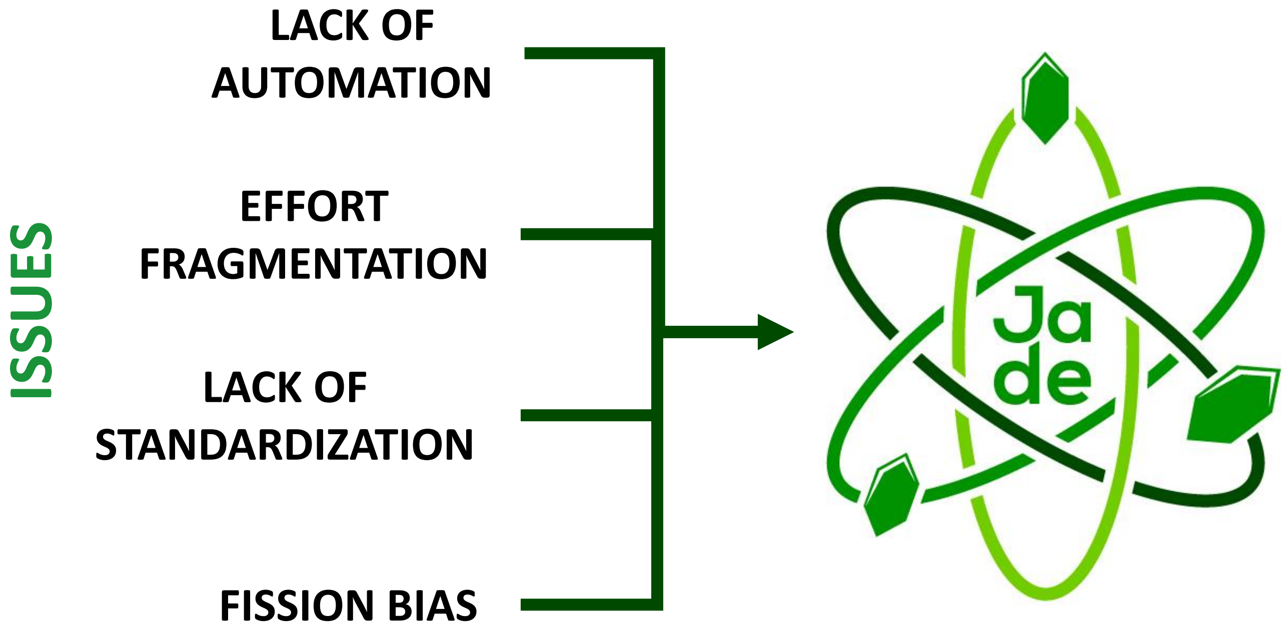
- complex geometries that need to be fully modelled
- different regions with different needs
- a detailed spatial distribution of tallies is needed

Vast amount of tallies and energy/spatial discretization

What is JADE?

JADE

JADE is a python based software that aims to establish itself as a corner stone for a complete and extensive **automated and standardized V&V procedure** for nuclear data libraries, with a special focus towards fusion applications.



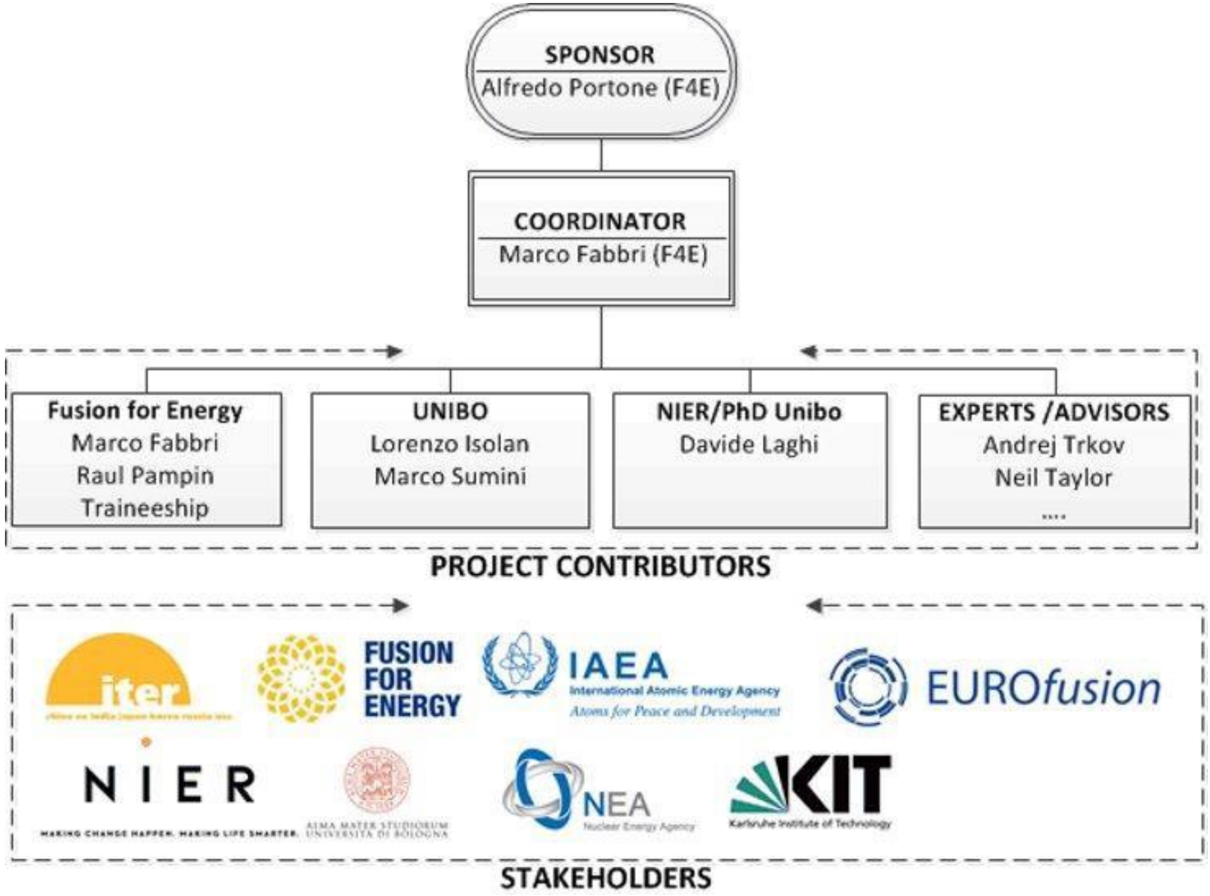
NIER
MAKING CHANGE HAPPEN. MAKING LIFE SMARTER.

ALMA MATER STUDIORUM A.D. 1088 UNIVERSITÀ DI BOLOGNA
DIPARTIMENTO DI INGEGNERIA INDUSTRIALE

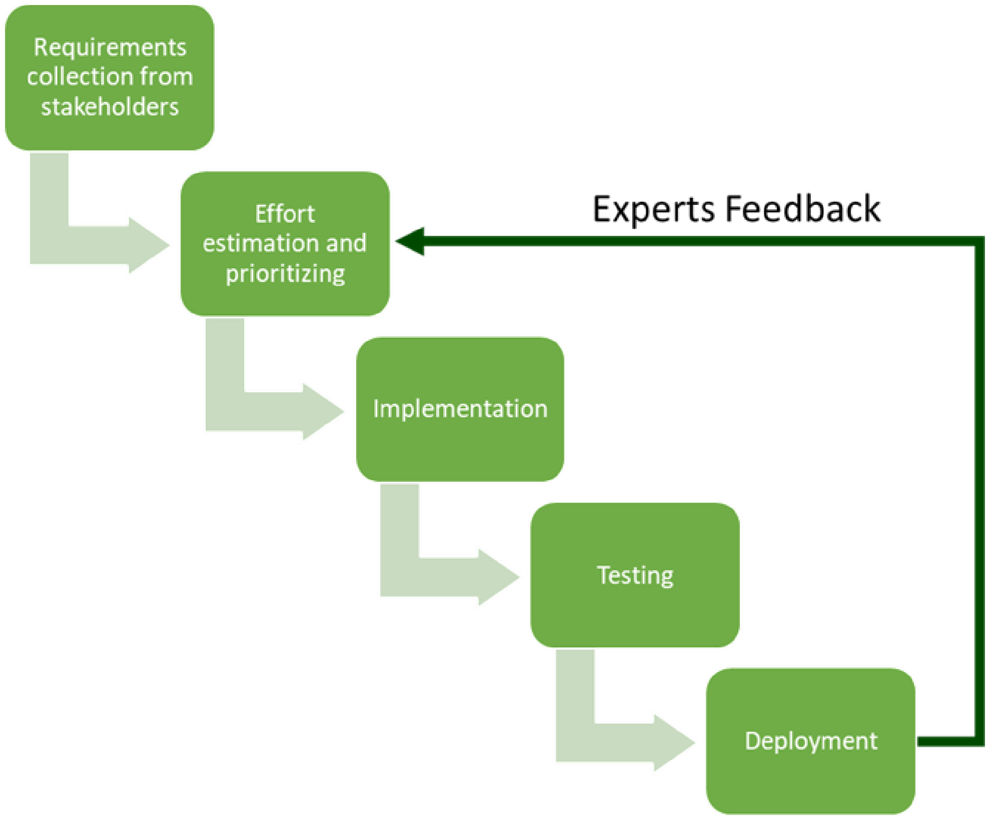
FUSION FOR ENERGY

What is JADE?

The organization of the project



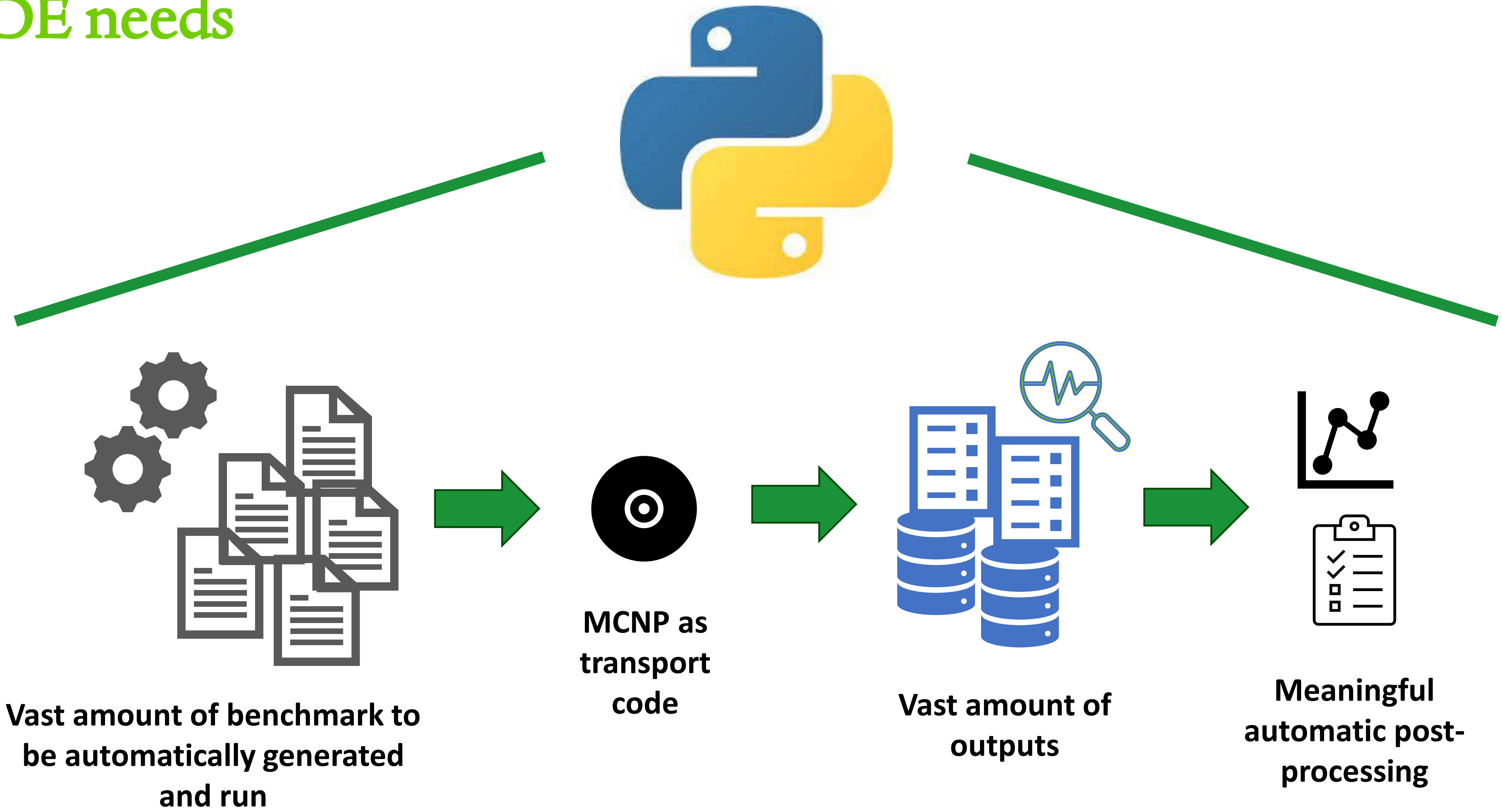
Waterfall approach



Implemented by means of a stage approach and > 1.5 ppy of total effort

What is JADE?

JADE needs



What is JADE?

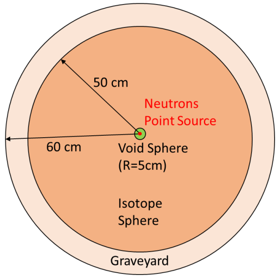
Benchmarks suite

TRANSPORT

ACTIVATION

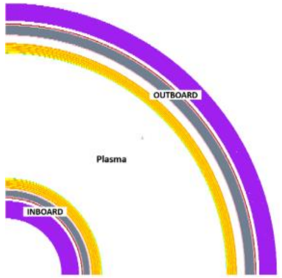
COMPUTATIONAL

Sphere Leakage

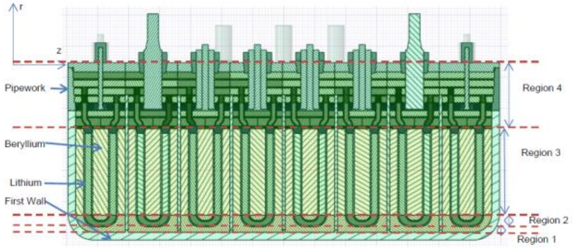


C-model

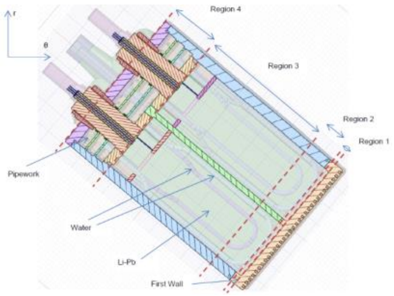
ITER 1D



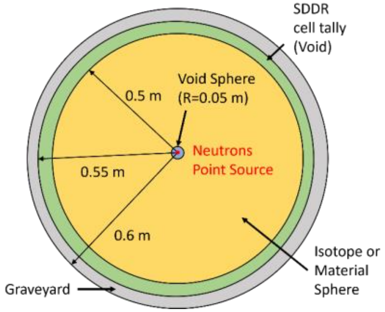
HCPB TBM



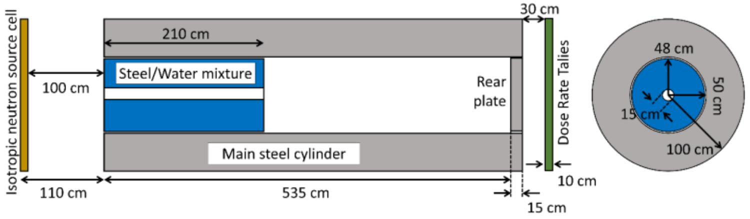
WCLL TBM



SPHERE SDDR

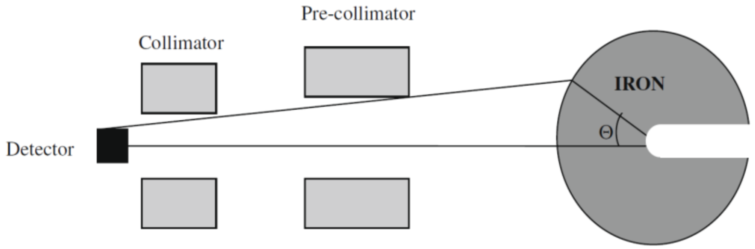


ITER CYL SDDR

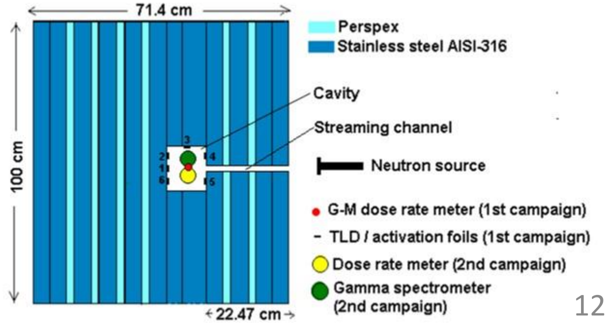


EXPERIMENTAL

OKTAVIAN

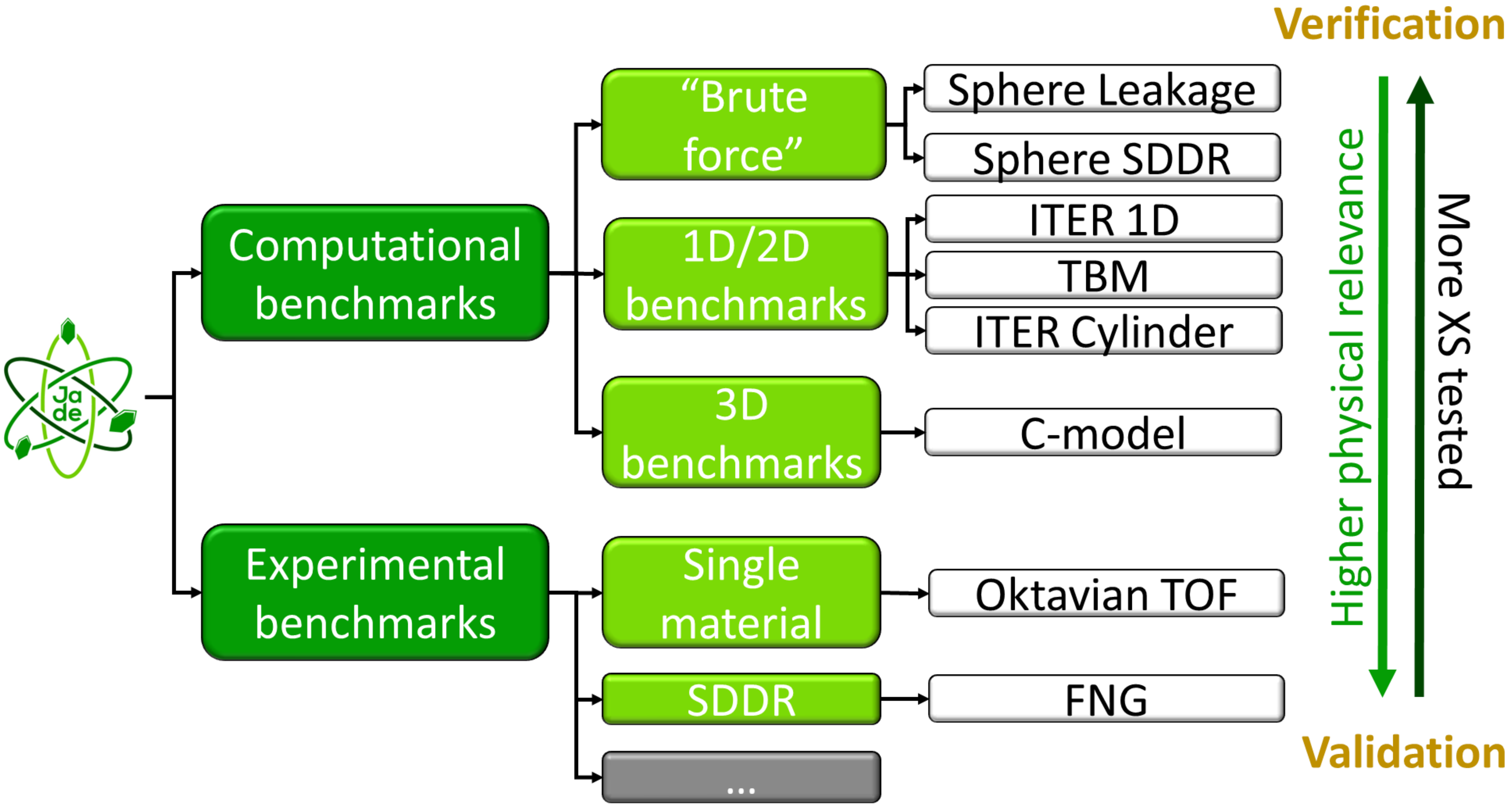


FNG SDDR



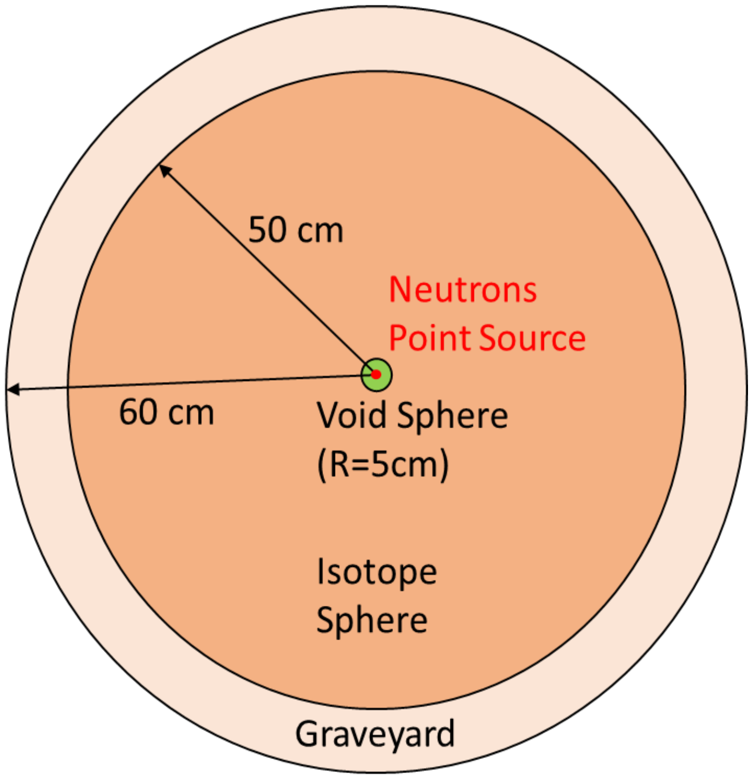
What is JADE

Benchmarks suite



The Sphere Leakage benchmark

Benchmark description



A uniform 0-14 MeV neutron point source is inserted at the center of a sphere composed entirely by a single isotope or a typical ITER material.

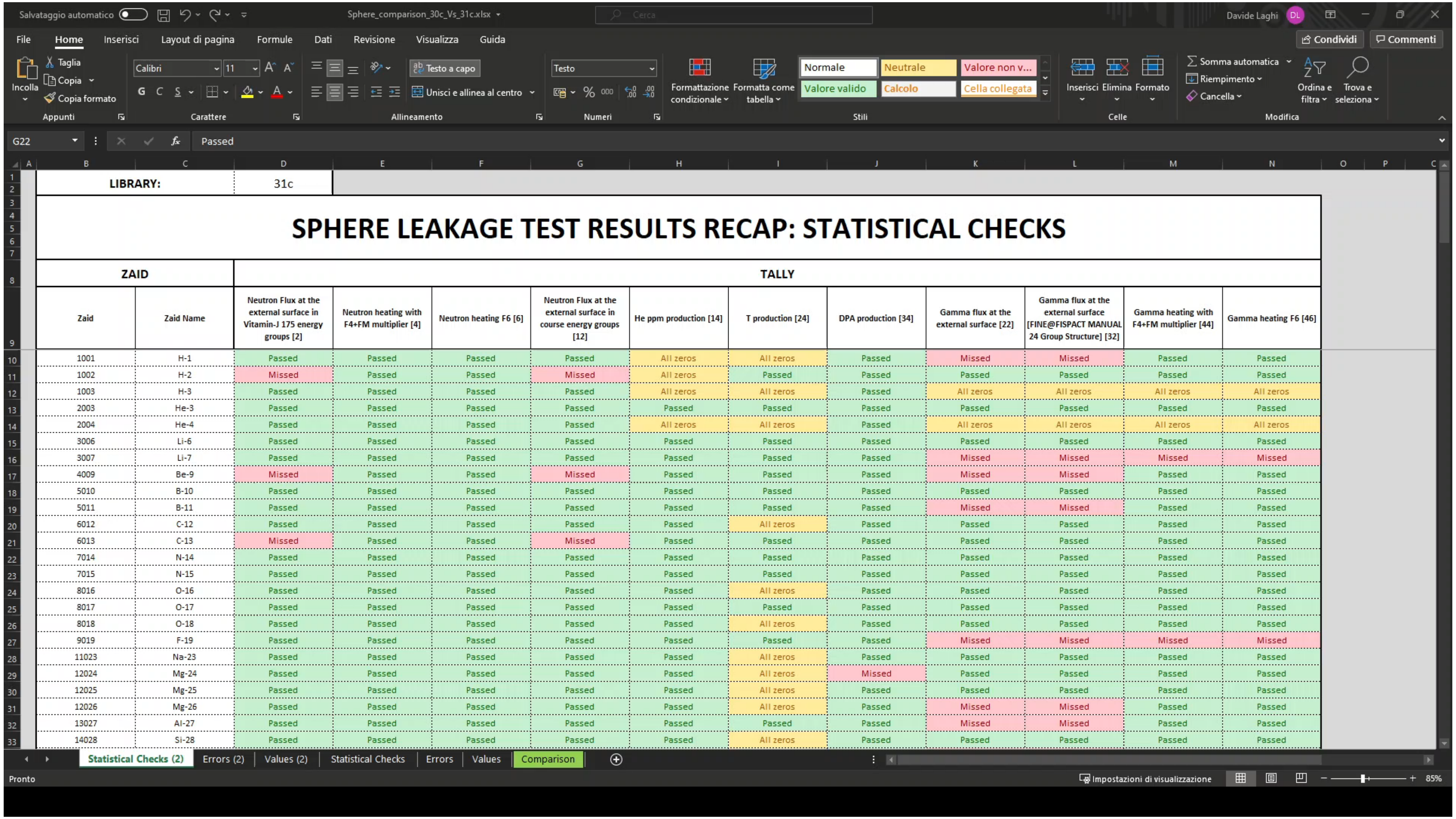
All isotopes provided by the nuclear data library under assessment are singularly tested.

Tallied quantities:

- Neutron and photon leakage flux (energy binned);
- Neutron and photon heating inside the sphere;
- Tritium and Helium production inside the sphere;
- DPA.

The Sphere Leakage benchmark

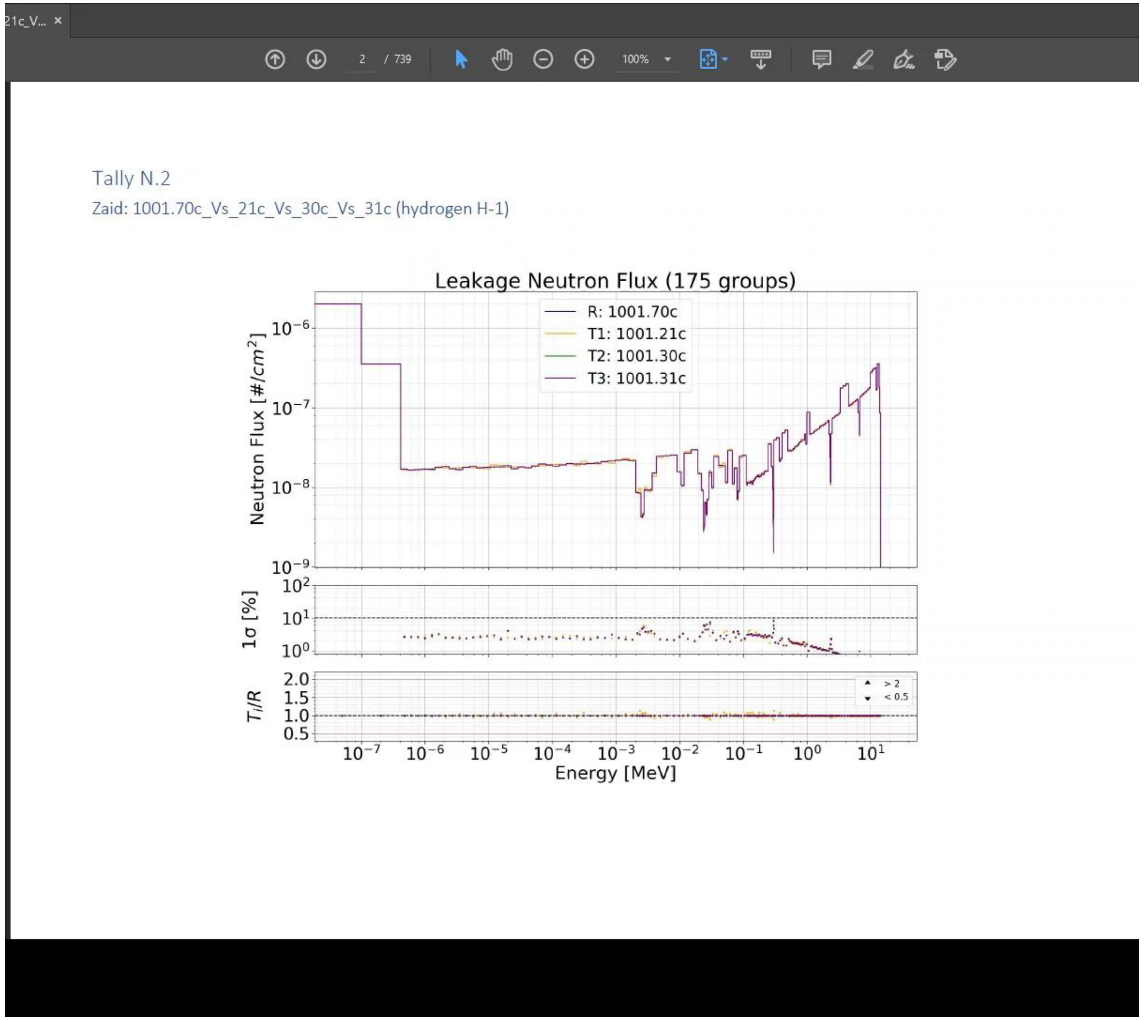
Excel formatted tables

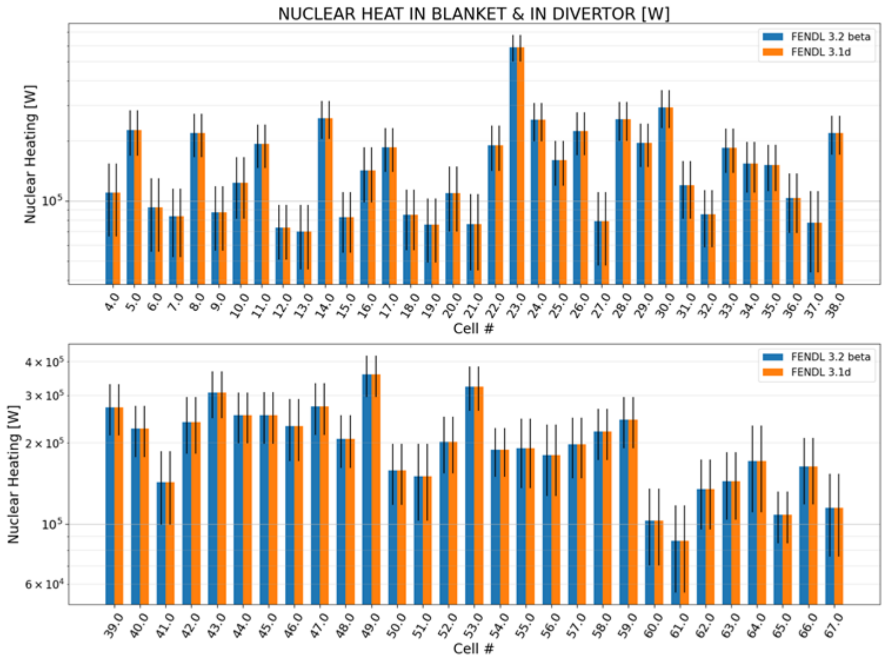


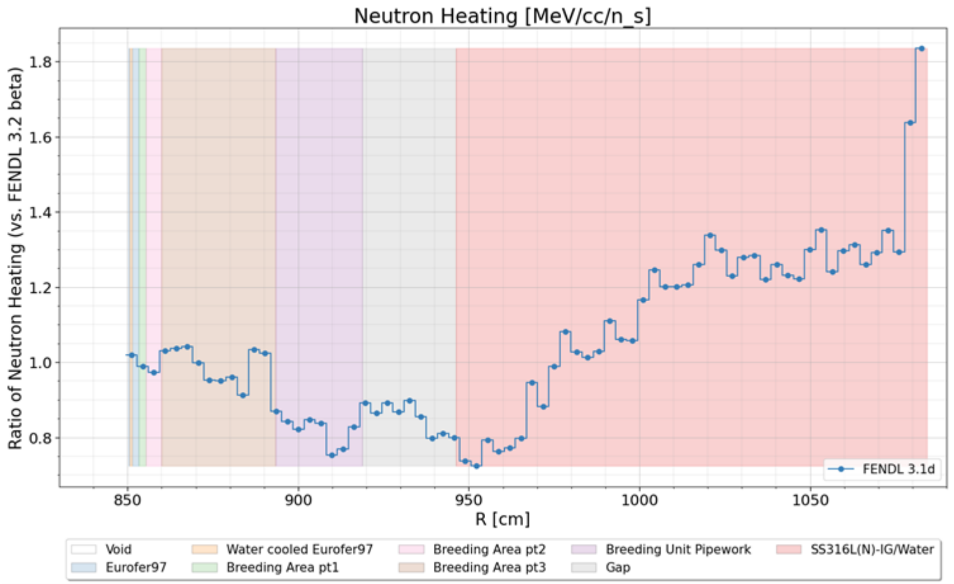
LIBRARY:	31c											
SPHERE LEAKAGE TEST RESULTS RECAP: STATISTICAL CHECKS												
ZAID		**TALLY**										
Zaid	Zaid Name	Neutron Flux at the external surface in Vitamin-J 175 energy groups [2]	Neutron heating with F4+FM multiplier [4]	Neutron heating F6 [6]	Neutron Flux at the external surface in course energy groups [12]	He ppm production [14]	T production [24]	DPA production [34]	Gamma flux at the external surface [22]	Gamma flux at the external surface [FINE@FISPACT MANUAL 24 Group Structure] [32]	Gamma heating with F4+FM multiplier [44]	Gamma heating F6 [46]
1001	H-1	Passed	Passed	Passed	Passed	All zeros	All zeros	Passed	Missed	Missed	Passed	Passed
1002	H-2	Missed	Passed	Passed	Missed	All zeros	Passed	Passed	Passed	Passed	Passed	Passed
1003	H-3	Passed	Passed	Passed	Passed	All zeros	All zeros	Passed	All zeros	All zeros	All zeros	All zeros
2003	He-3	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed
2004	He-4	Passed	Passed	Passed	Passed	All zeros	All zeros	Passed	All zeros	All zeros	All zeros	All zeros
3006	Li-6	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed
3007	Li-7	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Missed	Missed	Missed	Missed
4009	Be-9	Missed	Passed	Passed	Missed	Passed	Passed	Passed	Missed	Missed	Passed	Passed
5010	B-10	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed
5011	B-11	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Missed	Missed	Passed	Passed
6012	C-12	Passed	Passed	Passed	Passed	Passed	All zeros	Passed	Passed	Passed	Passed	Passed
6013	C-13	Missed	Passed	Passed	Missed	Passed	Passed	Passed	Passed	Passed	Passed	Passed
7014	N-14	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed
7015	N-15	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed
8016	O-16	Passed	Passed	Passed	Passed	Passed	All zeros	Passed	Passed	Passed	Passed	Passed
8017	O-17	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed
8018	O-18	Passed	Passed	Passed	Passed	Passed	All zeros	Passed	Passed	Passed	Passed	Passed
9019	F-19	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Missed	Missed	Missed	Missed
11023	Na-23	Passed	Passed	Passed	Passed	Passed	All zeros	Passed	Passed	Passed	Passed	Passed
12024	Mg-24	Passed	Passed	Passed	Passed	Passed	All zeros	Missed	Passed	Passed	Passed	Passed
12025	Mg-25	Passed	Passed	Passed	Passed	Passed	All zeros	Passed	Passed	Passed	Passed	Passed
12026	Mg-26	Passed	Passed	Passed	Passed	Passed	All zeros	Passed	Missed	Missed	Passed	Passed
13027	Al-27	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Missed	Missed	Passed	Passed
14028	Si-28	Passed	Passed	Passed	Passed	Passed	All zeros	Passed	Passed	Passed	Passed	Passed

The Sphere Leakage benchmark

Plot atlas

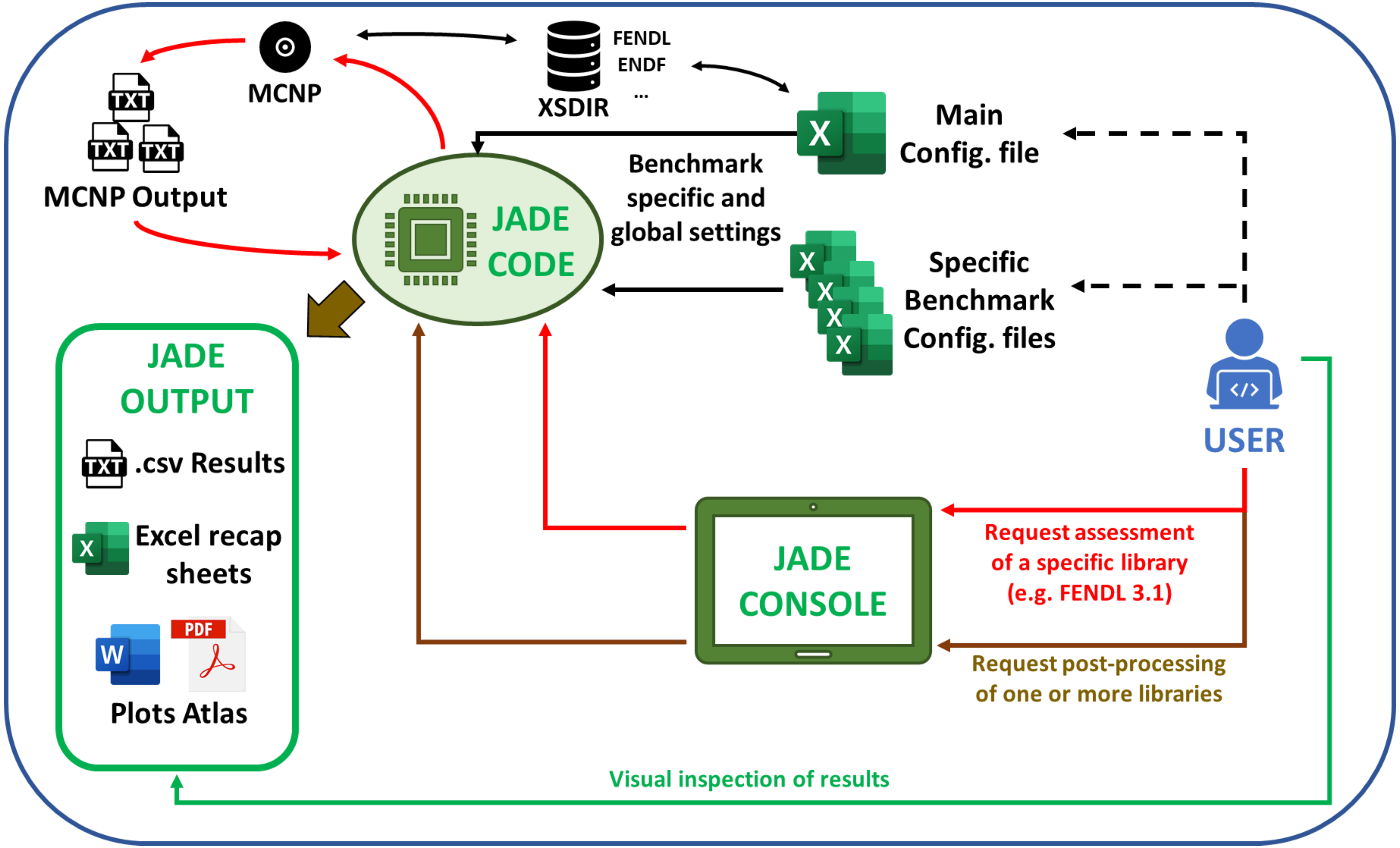






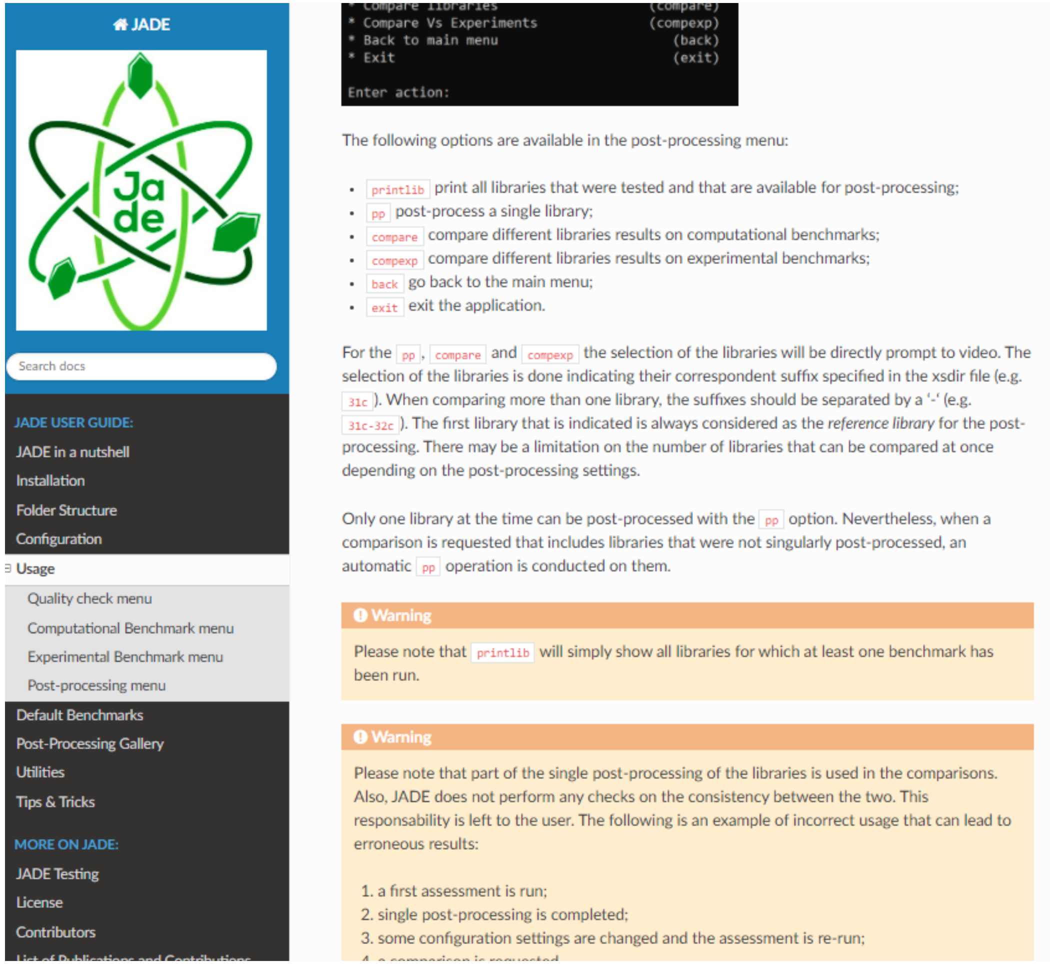
JADE architecture and development

General scheme

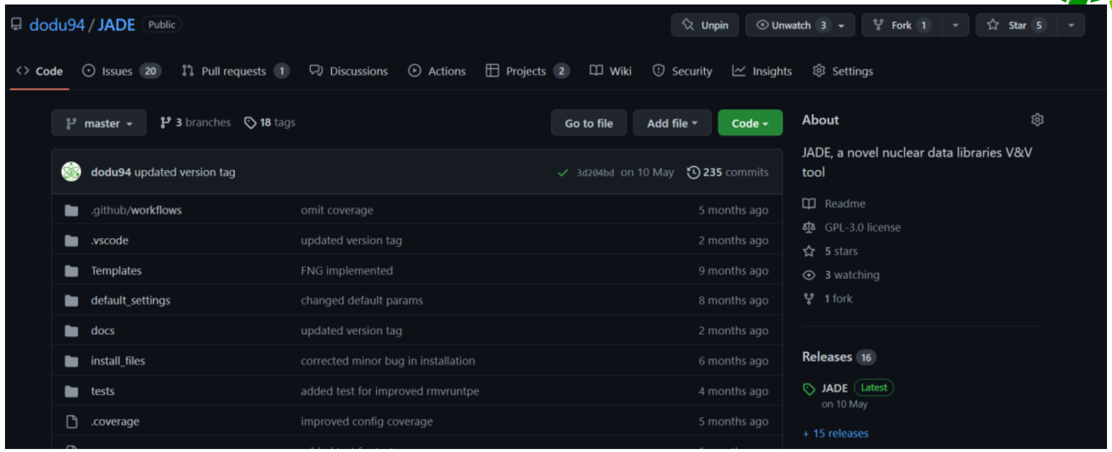


JADE Architecture and development

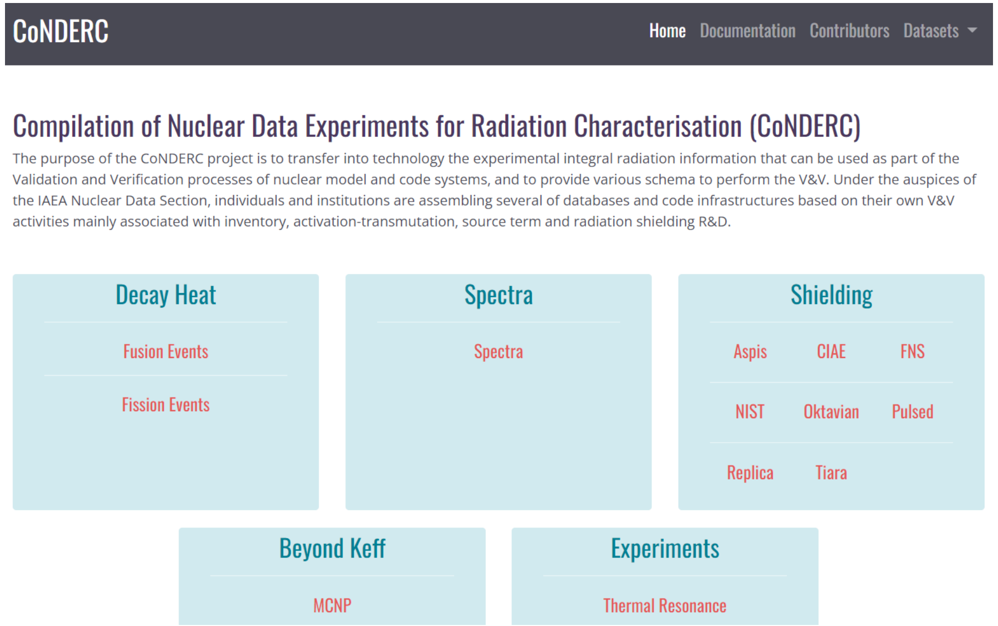
Open source



ReadTheDocs: https://jade-a-nuclear-data-libraries-vv-tool.readthedocs.io/en/latest/



GitHub: https://github.com/dodu94/JADE



CoNDERC: https://nds.iaea.org/conderc/

JADE architecture and development

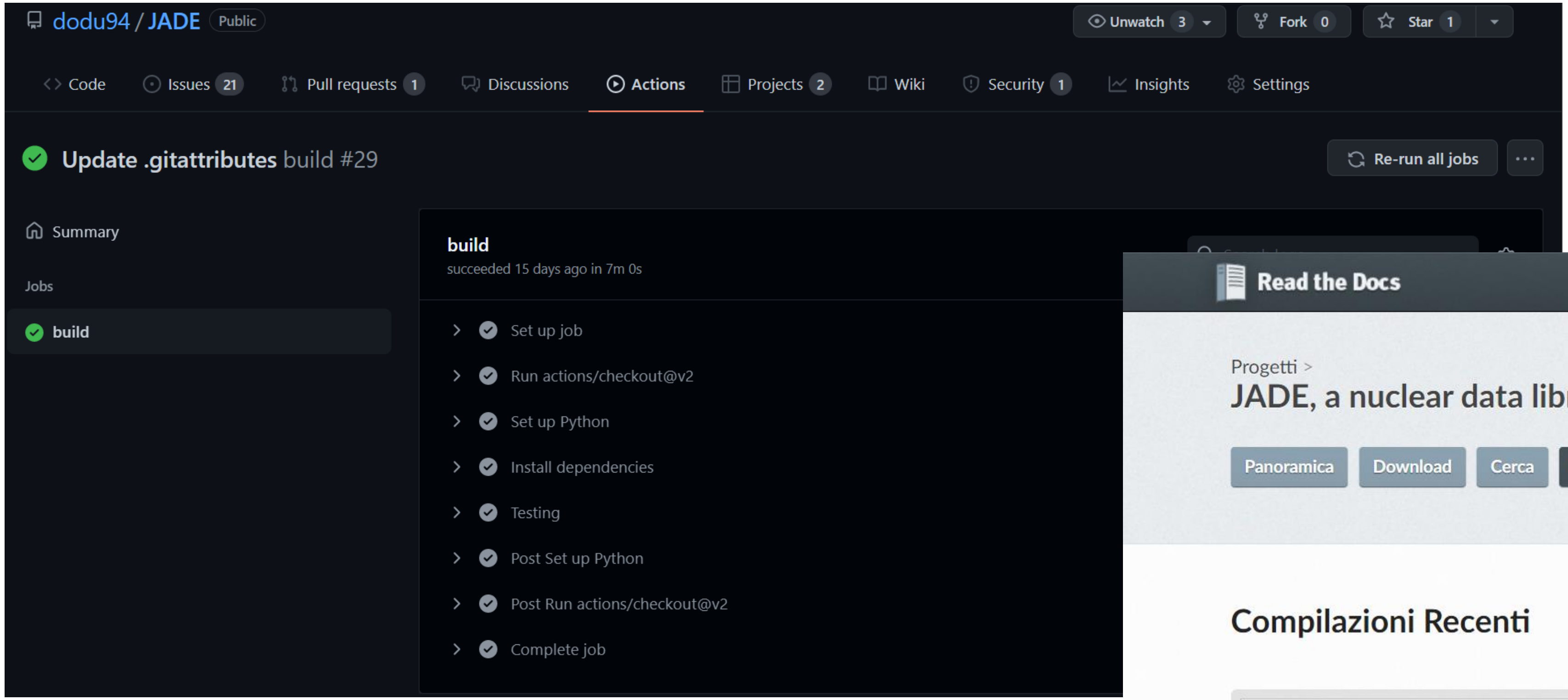
Automatic testing with pytest and coverage

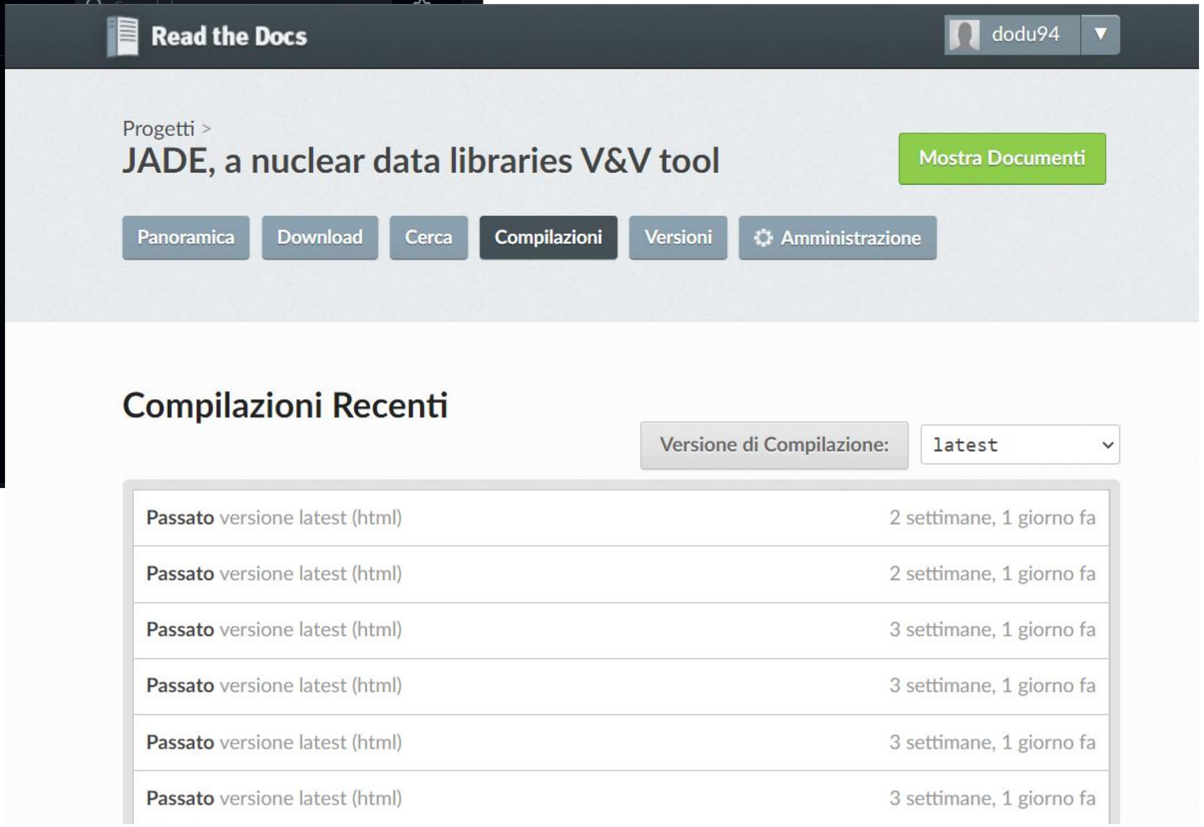
```
(base) C:\Users\d.laghi\Documents\GitHub\JADE\Code\tests>pytest
================================================= test session starts =================================================
platform win32 -- Python 3.8.5, pytest-6.1.1, py-1.9.0, pluggy-0.13.1
rootdir: C:\Users\d.laghi\Documents\GitHub\JADE\Code\tests
collected 29 items

inputfile_test.py ...                                                                                            [ 10%]
libmanager_test.py ....                                                                                          [ 24%]
matreader_test.py ......                                                                                         [ 44%]
output_test.py .                                                                                                 [ 48%]
parsersD1S_test.py .............                                                                                 [ 93%]
sphereoutput_test.py ..                                                                                          [100%]

================================================== warnings summary ===================================================
..\..\..\..\..\Anaconda3\lib\site-packages\pyreadline\py3k_compat.py:8
  C:\Users\d.laghi\Anaconda3\lib\site-packages\pyreadline\py3k_compat.py:8: DeprecationWarning: Using or importing the ABCs from 'collections' instead of from 'collectio
ns.abc' is deprecated since Python 3.3, and in 3.9 it will stop working
    return isinstance(x, collections.Callable)

..\..\..\..\..\Anaconda3\lib\site-packages\win32\lib\pywintypes.py:2
  C:\Users\d.laghi\Anaconda3\lib\site-packages\win32\lib\pywintypes.py:2: DeprecationWarning: the imp module is deprecated in favour of importlib; see the module's docum
entation for alternative uses
    import imp, sys, os

..\..\..\..\..\Anaconda3\lib\site-packages\docx\section.py:7
  C:\Users\d.laghi\Anaconda3\lib\site-packages\docx\section.py:7: DeprecationWarning: Using or importing the ABCs from 'collections' instead of from 'collections.abc' is
 deprecated since Python 3.3, and in 3.9 it will stop working
    from collections import Sequence

..\..\..\..\..\Anaconda3\lib\site-packages\xlrd\xlsx.py:266
..\..\..\..\..\Anaconda3\lib\site-packages\xlrd\xlsx.py:266
  C:\Users\d.laghi\Anaconda3\lib\site-packages\xlrd\xlsx.py:266: DeprecationWarning: This method will be removed in future versions.  Use 'tree.iter()' or 'list(tree.ite
r())' instead.
    for elem in self.tree.iter() if Element_has_iter else self.tree.getiterator():

..\..\..\..\..\Anaconda3\lib\site-packages\xlrd\xlsx.py:312
  C:\Users\d.laghi\Anaconda3\lib\site-packages\xlrd\xlsx.py:312: DeprecationWarning: This method will be removed in future versions.  Use 'tree.iter()' or 'list(tree.ite
r())' instead.
    for elem in self.tree.iter() if Element_has_iter else self.tree.getiterator():

matreader_test.py::TestMatCardList::test_translation
  ..\libmanager.py:162: UserWarning:  The Deafult library 81c was used for zaid 1001
    warnings.warn(MSG_DEFLIB.format(self.defaultlib, zaid))

-- Docs: https://docs.pytest.org/en/stable/warnings.html
=========================================== 29 passed, 7 warnings in 2.83s ============================================
```

- Help the stability of the code
- Increase trust on JADE results
- Sets a minimum quality standard for future contributors to the code
- Speed up introduction of new features (faster verification)

JADE architecture and development

Continuous Integration (CI)





At each push on the main JADE branch:

- JADE is installed in a cloud Windows environment and the automatic testing is run (handled by GitHub)
- The documentation is rebuilt by ReadTheDocs and adjourned

JADE in numbers

12k Lines of code

9 Implemented benchmarks

2 Published papers

D. Laghi et al, 2020, "JADE, a new software tool for nuclear fusion data libraries Verification & Validation", *Fusion Engineering and Design,* **161** 112075. DOI: https://doi.org/10.1016/j.fusengdes.2020.112075

D. Laghi et al, "Application of JADE V&V capabilities to the new FENDL v3.2 Beta release", *Nuclear Fusion*, **61** 11.DOI: http://iopscience.iop.org/article/10.1088/1741-4326/ac121a

$>10^6$ CPU simulation hours worth of data that has been post-processed

Looking ahead

Next foreseeable steps

Expansion of the benchmarks suite → **CoNDERC & SINBAD**

MCNP6 → OpenMC

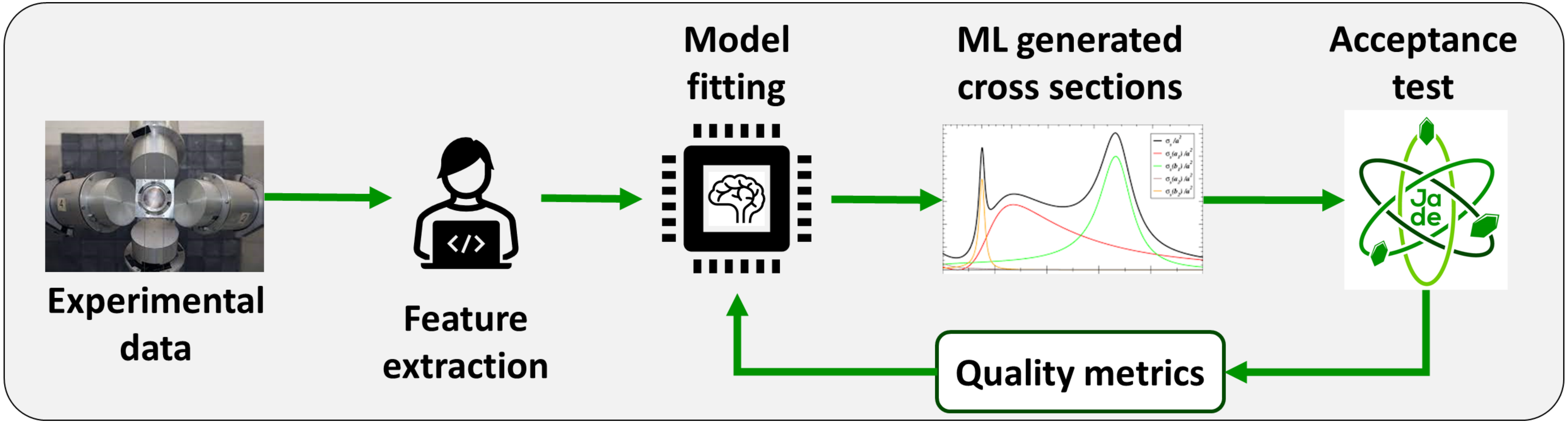
Windows → Linux

Machine learning: a possible mid-term future

Monte Carlo codes like OpenMC are currently porting their code to GPU solvers

Simulation time could decrease by a few order of magnitudes!

Leveraging the open source automation of benchmarks running and definition of acceptance test, ML algorithm could be introduced to support the libraries evaluation process



An example of application is **NucML**[1]: https://pedrojrv.github.io/nucml/index.html

[1]Pedro Jr. Vicente-Valdez, Massimiliano Fratoni (UC Berkely, USA)

What it will be great to have

- A comprehensive, unified, user-friendly, open-source, ready to be used database of experiment (e.g., Conderc+SINBAD GitHub).
- A platform to provide feedback and record exchanges (e.g., GitHub).
- A collection of computational benchmark to use (e.g., 1D ITER).
- A standardized way to share and collect the different executed benchmarks in a common database (e.g., CONDERC) trying to avoid duplication.
- A closer collaboration with the different parties with periodic exchange (i.e., CCFE).
- Guidelines for the V&V of (fusion) libraries with clear acceptance criteria (e.g., C/E TBR : [0.95, 1.05]).

Summary

- JADE improves the standardization and the automation level in the field of nuclear data V&V (especially regarding fusion application).
- JADE is a consolidated open-source tool built for the community by the community. If you are interested on collaborating do not hesitate to contact us. Let's join forces.
- V&V on many libraries has been already performed by JADE(i.e., FENDL3.1d, FENDL3.2, JEFF-3.3., JEFF-4.0T1). Few inconsistencies and discrepancies were spotted and reported. More work is planned.
- We sincerely appreciate the effort put in place by NEA, IAEA, SINBAD to modernize the experimental database and the collaboration with the different parties to continue the development of JADE.

GitHub: https://github.com/dodu94/JADE

READ THE DOCS: https://readthedocs.org/

Any Questions?

Thank you for your kind attention!

Powered By:

NIER

MAKING CHANGE HAPPEN. MAKING LIFE SMARTER.

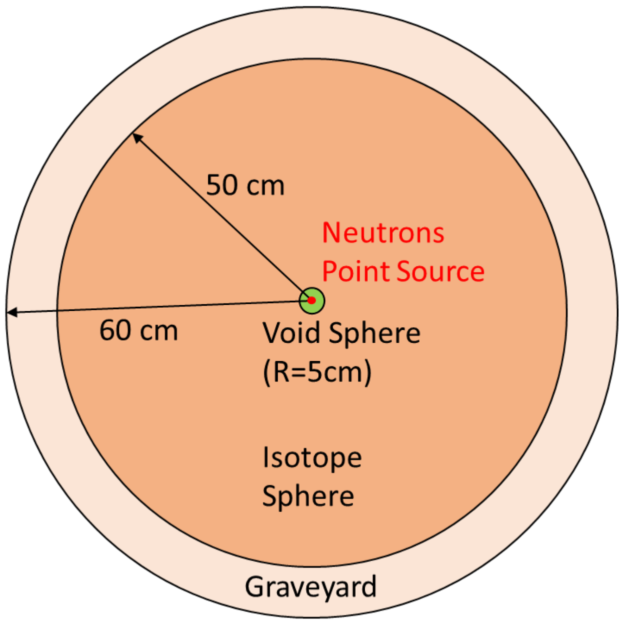
DIPARTIMENTO DI INGEGNERIA INDUSTRIALE

FUSION FOR ENERGY

Backup slides

JADE application to production cases

Proof of concept



Tested libraries:

- **FENDL v2.1**
- **FENDL v3.0**
- **FENDL v3.1d**
- **ENDF VII.1**

LIBRARY:	31c

SPHERE LEAKAGE TEST RESULTS RECAP: VALUES

ZAID		TALLY							
Zaid	Zaid Name	Neutron Flux at the external surface in Vitamin-J 175 energy groups	He ppm production	T production	DPA production	Gamma flux at the external surface [FINE@FISPACT MANUAL 24 Group Structure]	Neutron Heating comparison [F4 vs F6]	Gamma Heating comparison [F4 vs F6]	Notes
41093	Nb-93	Value > 0 for all bins	Value > 0 for all bins	Value = 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	0.00%	0.00%	
42092	Mo-92	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	69.37%	0.00%	
42094	Mo-94	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	326.49%	0.00%	
42095	Mo-95	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	270.14%	0.00%	
42096	Mo-96	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	309.40%	0.00%	
42097	Mo-97	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	228.12%	0.00%	
42098	Mo-98	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	206.98%	0.00%	
42100	Mo-100	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	269.58%	0.00%	
45103	Rh-103	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	145.85%	0.00%	
47107	Ag-107	Value > 0 for all bins	Value > 0 for all bins	Value = 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	0.00%	0.00%	
47109	Ag-109	Value > 0 for all bins	Value > 0 for all bins	Value = 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	0.00%	0.00%	
48106	Cd-106	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	0.00%	0.00%	
48108	Cd-108	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value = 0 for all bins	355.40%	0.00%	
48110	Cd-110	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value = 0 for all bins	222.39%	0.00%	
48111	Cd-111	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	0.00%	0.00%	
48112	Cd-112	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value = 0 for all bins	261.28%	0.00%	
48113	Cd-113	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value = 0 for all bins	182.22%	0.00%	
48114	Cd-114	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value = 0 for all bins	255.50%	0.00%	
48116	Cd-116	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value = 0 for all bins	215.38%	0.00%	
50112	Sn-112	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	0.00%	0.00%	
50114	Sn-114	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	0.00%	0.00%	
50115	Sn-115	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	0.00%	0.00%	
50116	Sn-116	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	0.00%	0.00%	

LEGEND	
(red)	>|5|%
(orange)	|1|% ≤ |5|%
(yellow)	|0.5|% ≤ |1|%
(green)	< |0.5|%

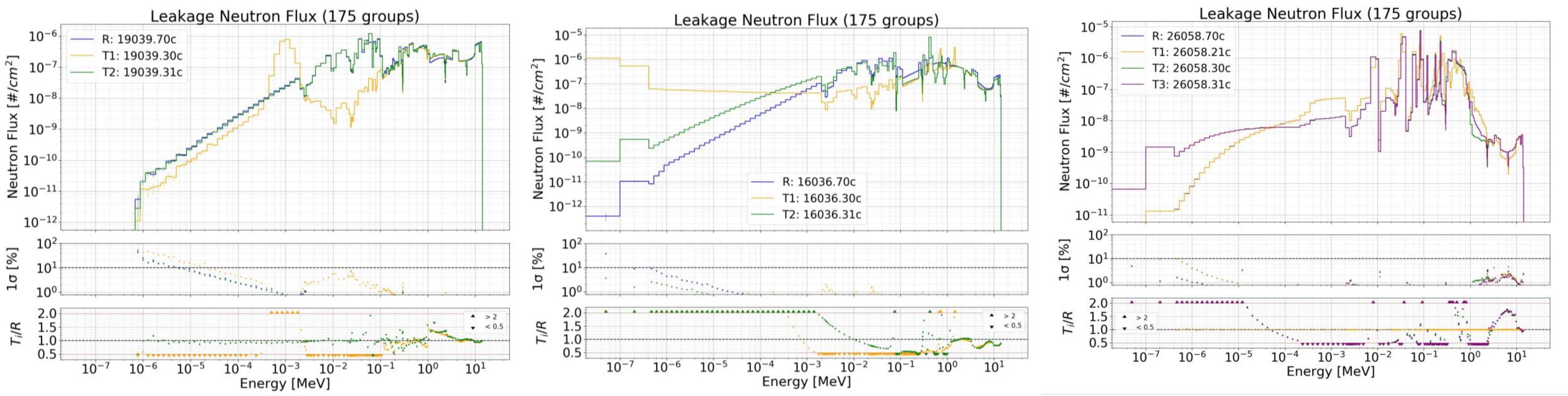
Known errors in the FENDL v3.1d were re-spotted by JADE consistency checks

Paper:

D. Laghi, M. Fabbri, L. Isolan, R. Pampin, M. Sumini, A. Portone and A. Trkov, 2020, “JADE, a new software tool for nuclear fusion data libraries Verification & Validation”, *Fusion Engineering and Design*, **161** 112075. DOI: https://doi.org/10.1016/j.fusengdes.2020.112075

JADE application to production cases

Proof of concept



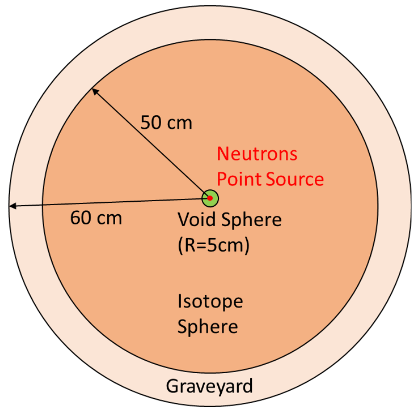
Some examples where the leakage neutron flux results differed significantly among the tested libraries.

JADE application to production cases

FENDL v3.2 release (BETA)

SPHERE LEAKAGE COMPARISON RECAP

ZAID		TALLIES				
		T production	He ppm production	DPA production	Neutron heating F6	Gamma heating F6
M901	Polyethylene, Non-borated		-0.01%	0.01%	0.02%	0.02%
M900	Natural silicon		0.00%	0.00%	0.00%	0.00%
M101	SS316L(N)-IG	0.57%	4.18%	**79.12%**	**98.41%**	2.38%
M203	Boron carbide (B_4C)	9.68%	0.79%	**100.00%**	**100.00%**	-0.01%
M200	Ordinary concrete	1.52%	10.47%	**87.15%**	**97.53%**	-8.15%
M400	Water	0.57%	16.37%	-2.82%	6.00%	-3.24%



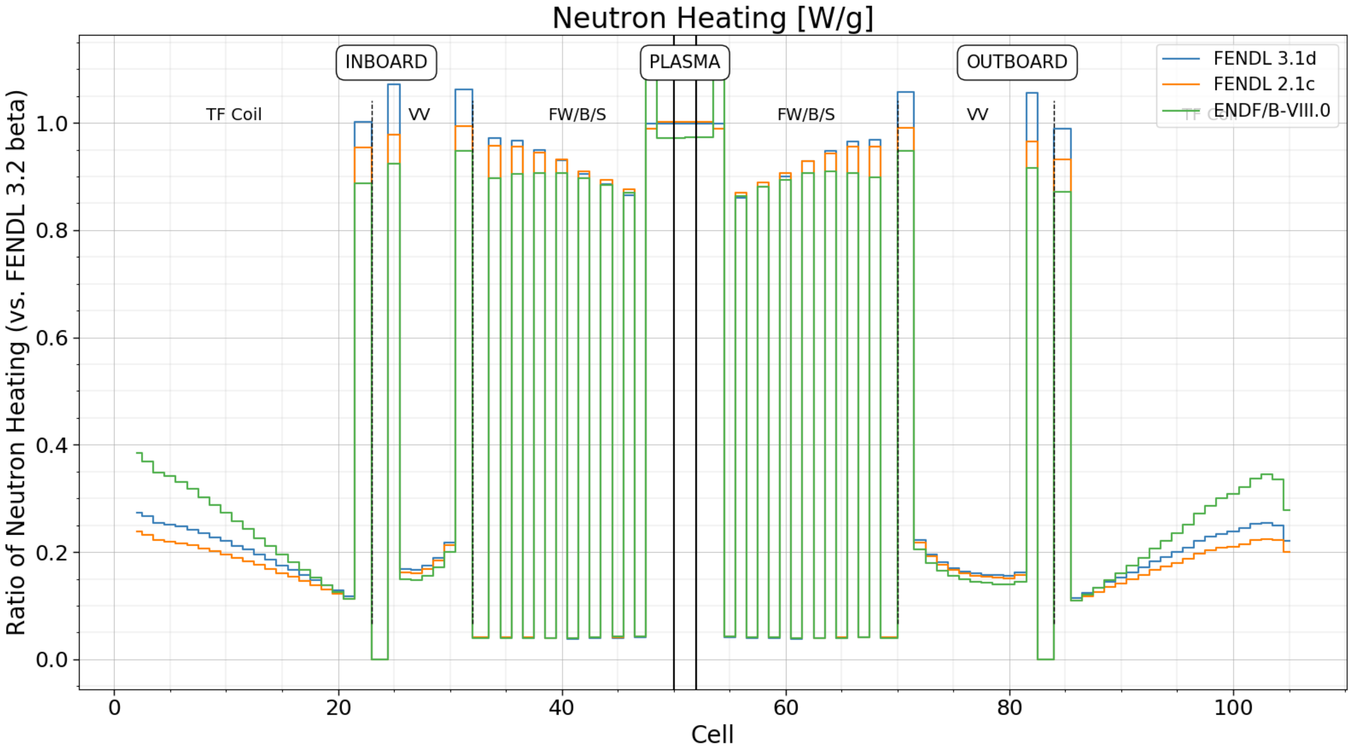
Important differences in key neutron related quantities were spotted for typical ITER materials when comparing the old and new release of FENDL libraries

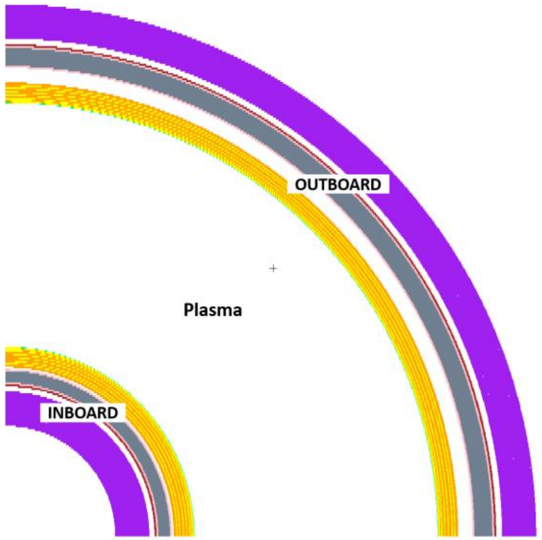
Paper:

D. Laghi, M. Fabbri, L. Isolan, M. Sumini, G. Schnabel and A. Trkov, 2021, "Application of JADE V&V capabilities to the new FENDL v3.2 Beta release", *Nuclear Fusion*, **61** 11.DOI: http://iopscience.iop.org/article/10.1088/1741-4326/ac121a

JADE application to production cases

FENDL v3.2 release (BETA)





Effect of the higher neutron heating in the steel layers of the ITER 1D model

SPHERE LEAKAGE COMPARISON RECAP						
ZAID		TALLIES				
		T production	He ppm production	DPA production	Neutron heating F6	Gamma heating F6
5010	B-10	5.17%	0.49%	100.00%	100.00%	-0.50%

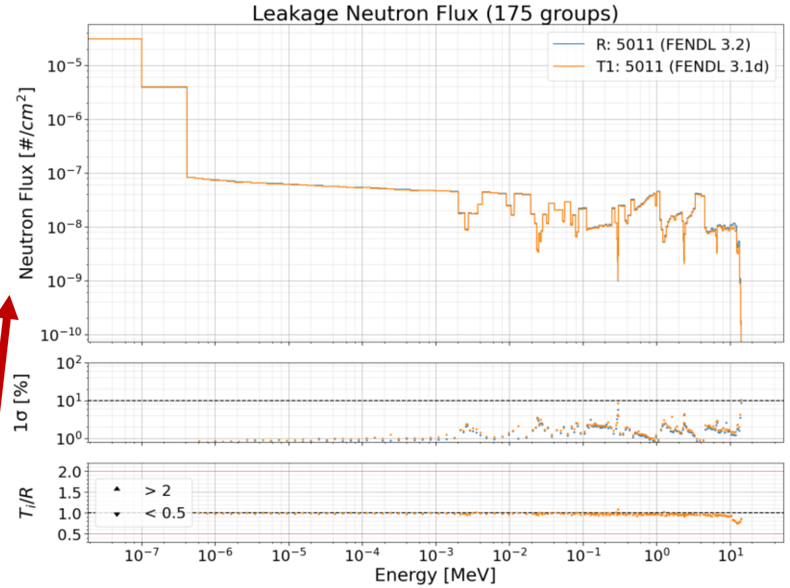
B-10 accounts only for 0.00036 % (in mass) of SS316L(N)-IG and at the same time SS316L(N)-IG is composed by 45 different isotopes. Without systematic and automated testing it would have been more difficult to track the origin of the issue.

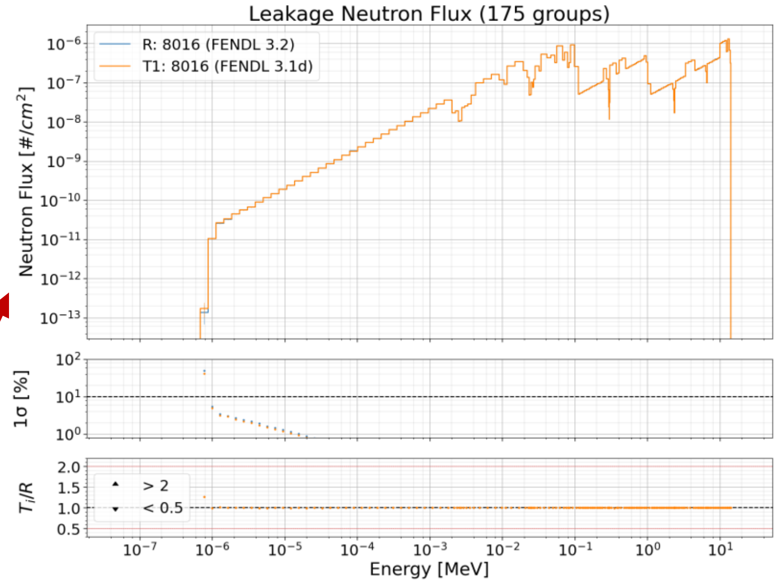
JADE application to production cases

FENDL v3.2 official release

ZAID		TALLIES				
Zaid N.	Symbol	T production	He ppm production	DPA production	Neutron heating F6	Gamma heating F6
M101	SS316L(N)-IG	8.59%	0.57%	0.15%	-8.67%	3.92%
M200	Ordinary Concrete	-0.27%	3.09%	-0.42%	10.15%	-2.53%
M203	Boron Carbide	13.13%	0.80%	-0.09%	-1.28%	0.95%
M400	Water	1.10%	16.19%	-1.86%	6.52%	-2.35%
M900	Natural Silicon		0.00%	0.00%	0.00%	0.00%
M901	Polyethylene, non-borated		0.00%	0.01%	0.02%	0.01%

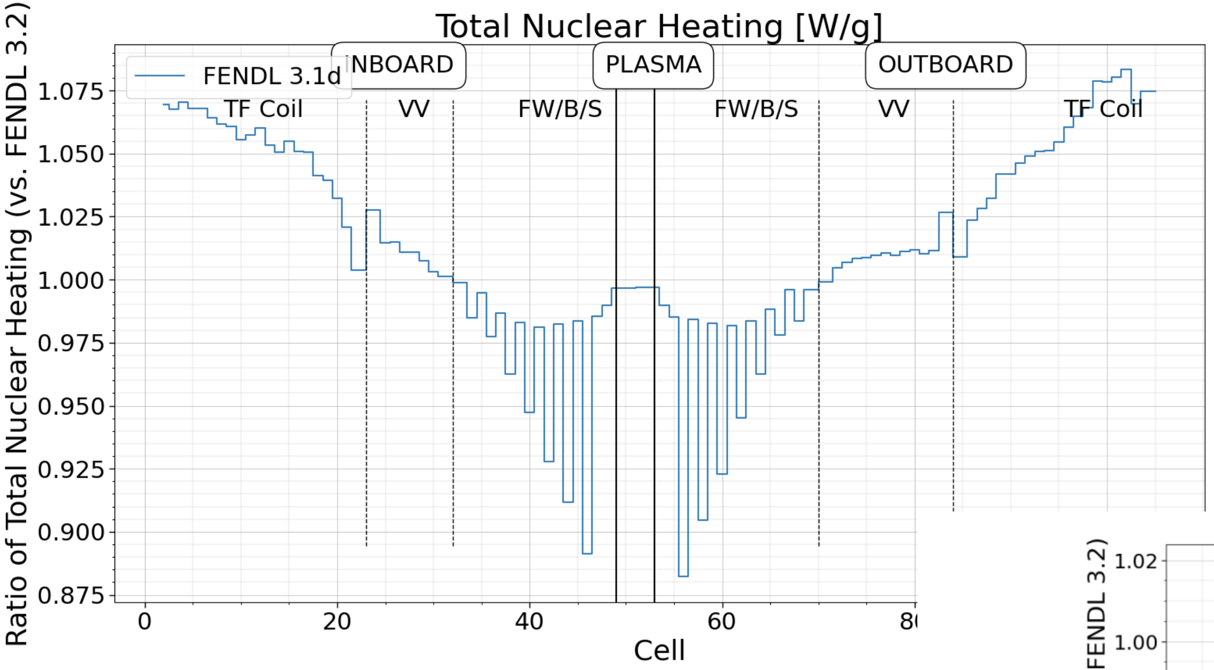
ZAID		TALLIES				
Zaid N.	Symbol	T production	He ppm production	DPA production	Neutron heating F6	Gamma heating F6
3007	Li-7	-0.01%	-0.01%	0.00%	-0.01%	-0.01%
4009	Be-9	0.04%	0.04%	0.02%	0.03%	-0.03%
5010	B-10	5.17%	0.49%	-2.55%	-6.53%	-0.50%
5011	B-11	39.56%	16.60%	0.24%	0.60%	1.46%
6012	C-12		-0.09%	0.04%	0.01%	-0.04%
6013	C-13	0.03%	-0.04%	0.02%	0.01%	-0.04%
7014	N-14	0.00%	0.00%	0.00%	0.00%	-0.01%
7015	N-15	0.00%	0.00%	0.00%	Identical	-0.01%
8016	O-16		17.63%	-3.09%	32.79%	-20.20%
8017	O-17	0.00%	0.00%	Identical	0.00%	-0.05%
8018	O-18		-91.74%	-35.81%	-12.19%	-47.58%





JADE application to production cases

FENDL v3.2 official release (Water/O-16)



Difference in neutron heating are clearly visible in water both in ITER1D and HCPB TBM benchmarks.

IAEA nuclear data section is considering for the O-16 cross section to either to:

- Switch to ENDFVIII.0 evaluation;
- Correct NJOY processing routine for KERMA data