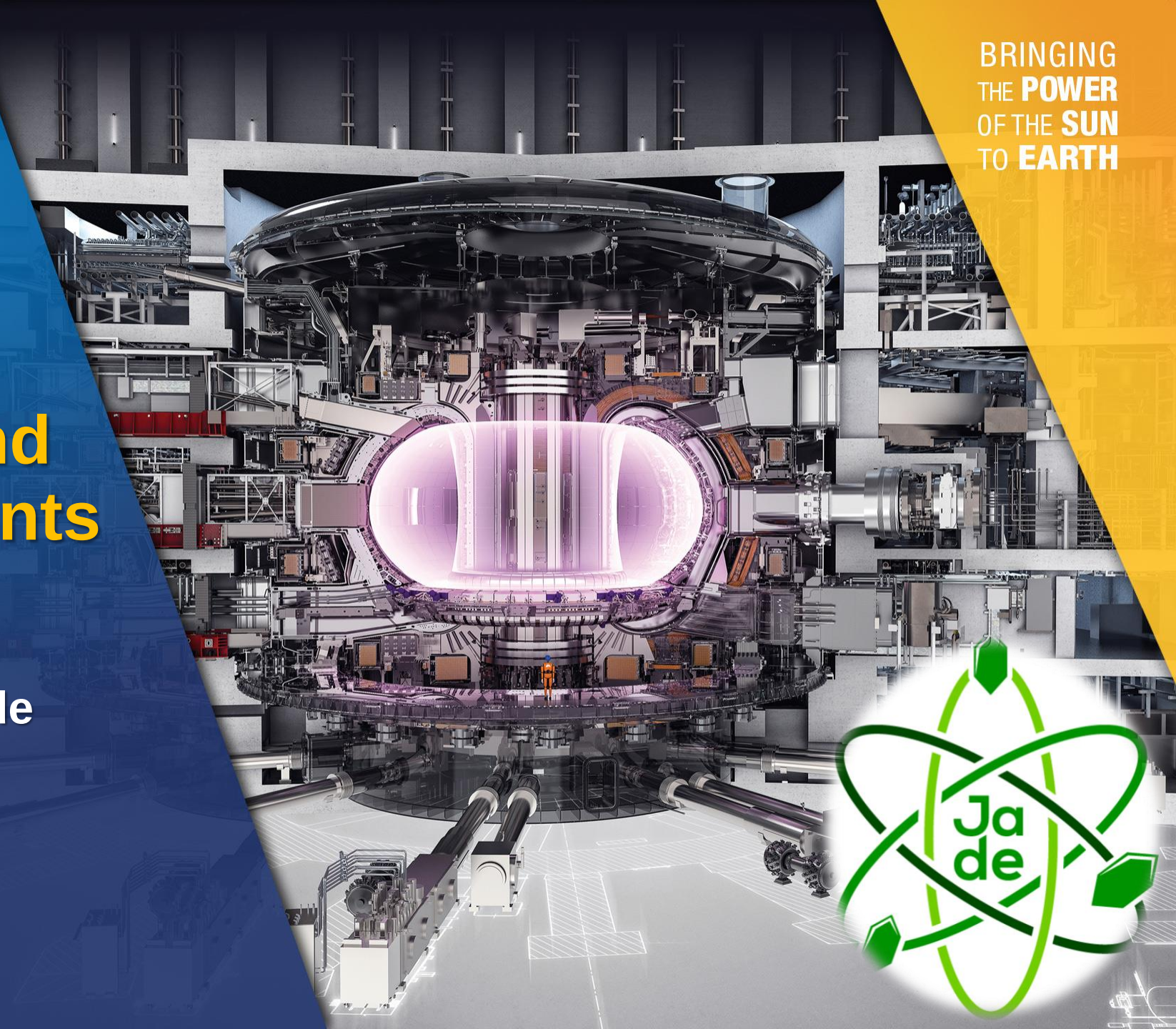
FUSION FOR ENERGY

BRINGING THE POWER OF THE SUN TO EARTH

Status of JADE and recent developments

Alberto Bittesnich, Davide Laghi*, Marco Fabbri*

01/11/2023



Outline

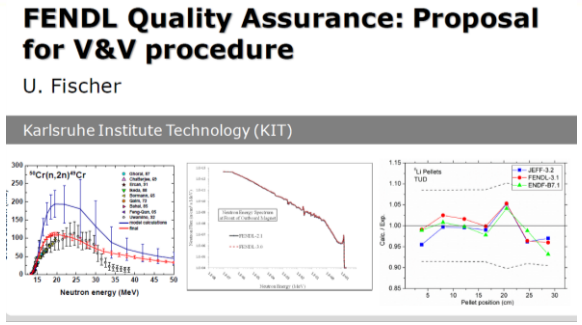
- Quick refresh: what is JADE
- Recent advancements on F4E side
- Recent advancements on UKAEA side*
- Looking ahead
- Conclusion

*Next presentation by Alex Valentine

Quick refresh: What is Jade

Why JADE?

Original proposal/idea from U. Fisher at 2018 IAEA FENDL consultants meeting



ISSUES

- LACK OF AUTOMATION
- EFFORT FRAGMENTATION
- LACK OF STANDARDIZATION
- FISSION BIAS

Jade

NIER
MAKING CHANGE HAPPEN. MAKING LIFE SMARTER.

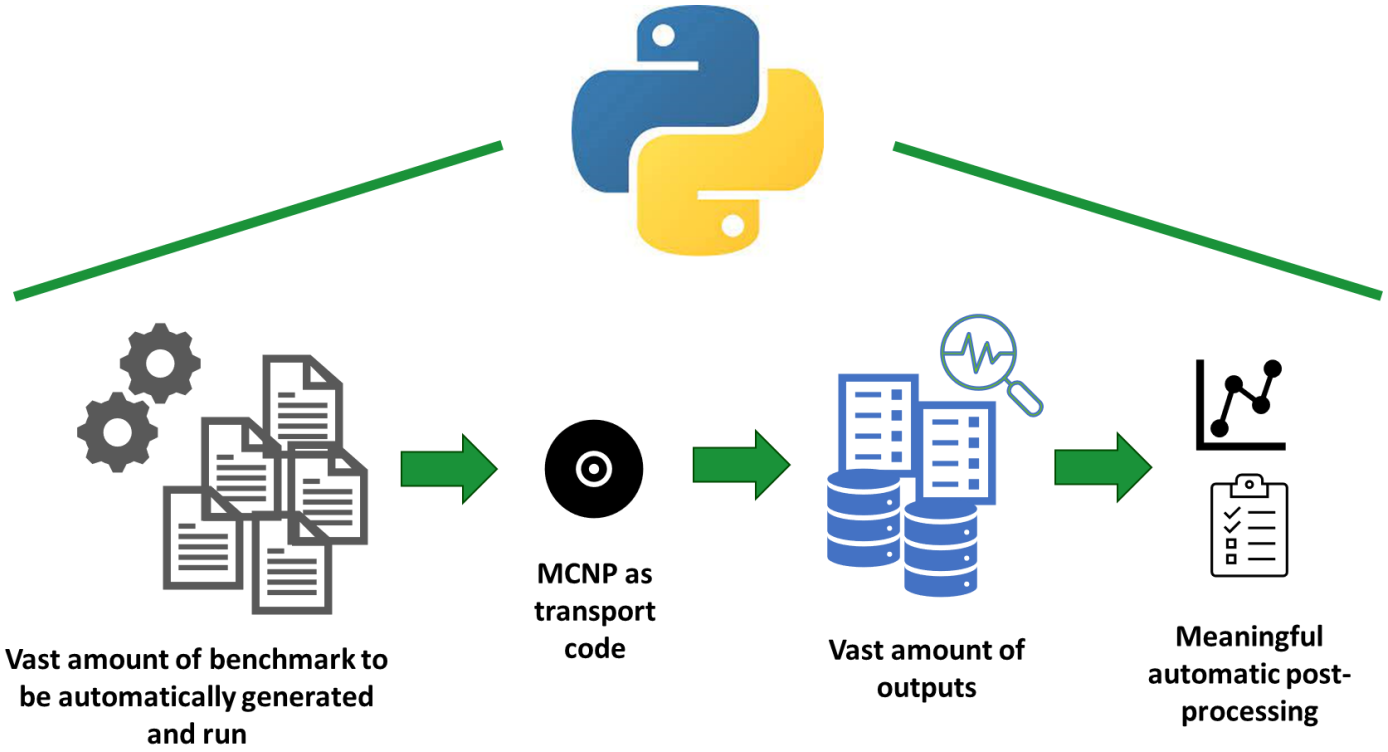
ALMA MATER STUDIORUM A.D. 1088
DIPARTIMENTO DI INGEGNERIA INDUSTRIALE

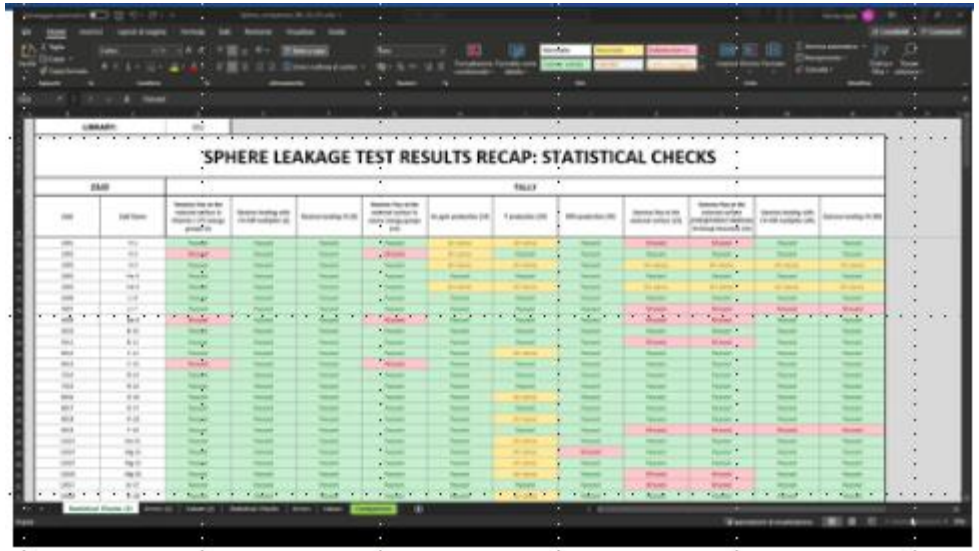
UK Atomic Energy Authority

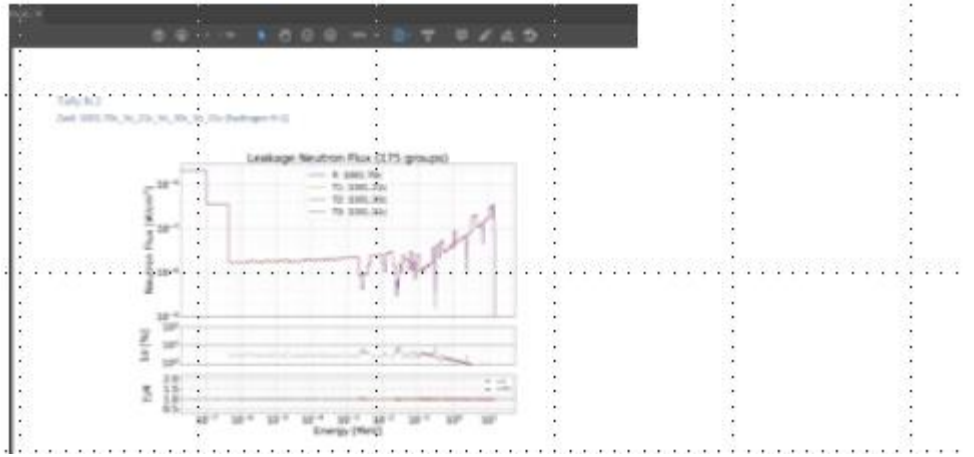
FUSION FOR ENERGY

Jožef Stefan Institute

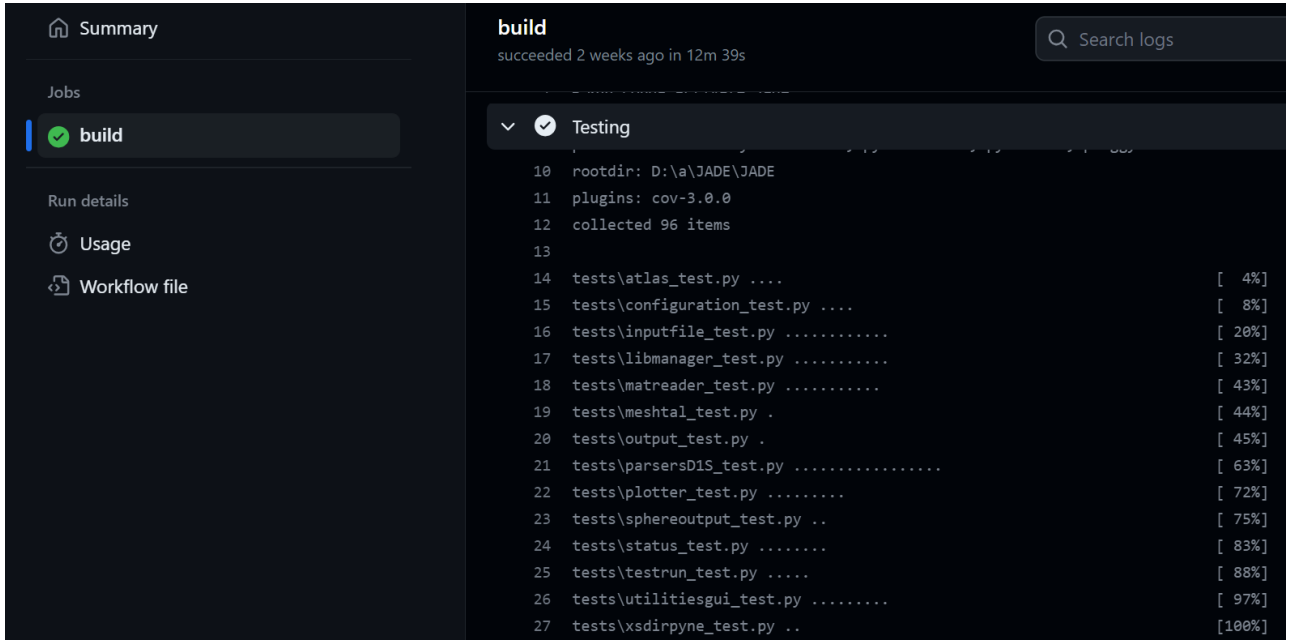
What is JADE?

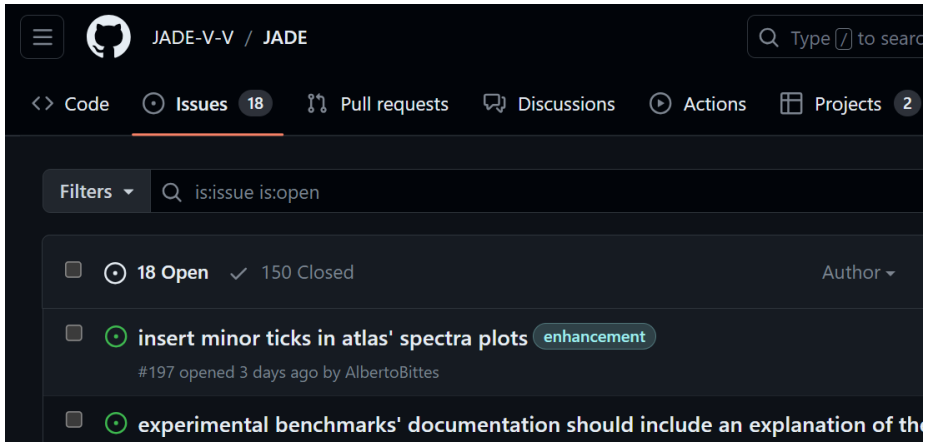

Vast amount of benchmark to be automatically generated and run
MCNP as transport code
Vast amount of outputs
Meaningful automatic post-processing

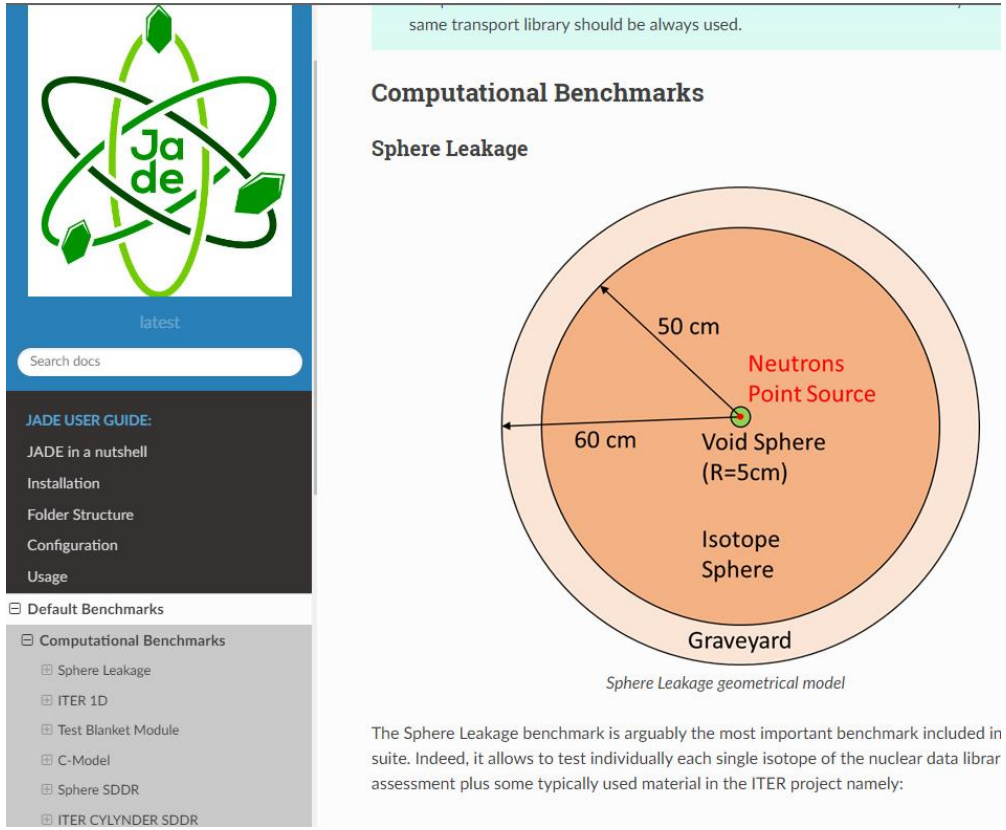

SPHERE LEAKAGE TEST RESULTS RECAP: STATISTICAL CHECKS



Continuous Integration







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

13k Lines of code

15 Implemented benchmarks

4 Published papers

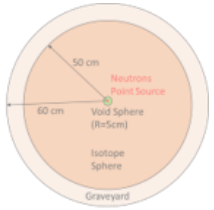
$>10^7$ CPU simulation hours worth of data that has been post-processed

Recent advancements on F4E side

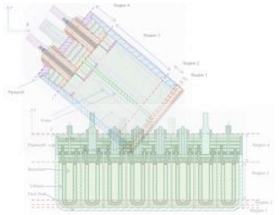
Benchmarks status

TRANSPORT

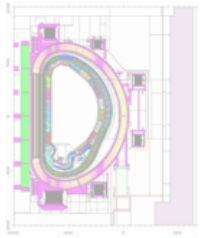
COMPUTATIONAL



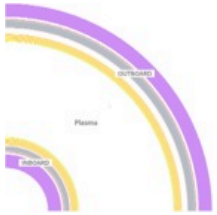
Sphere Leakage



WCLL & HCPB TBM

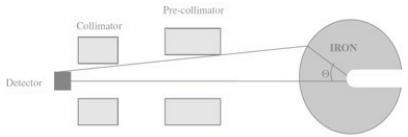


C-Model

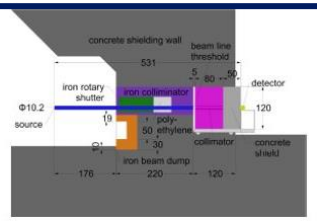


ITER-1D

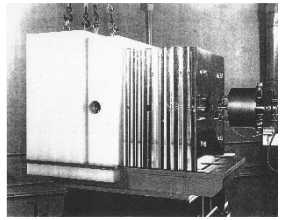
EXPERIMENTAL



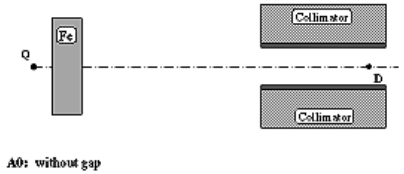
Oktavian



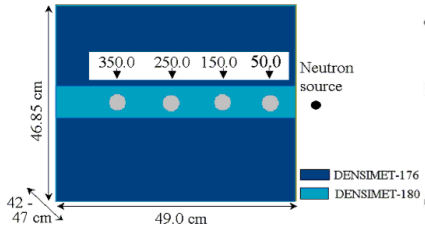
TIARA



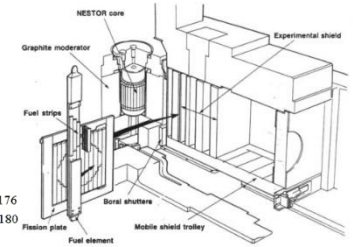
FNG Bulk Blanket



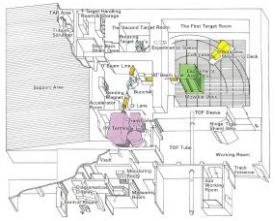
TUD Fe slab



FNG W

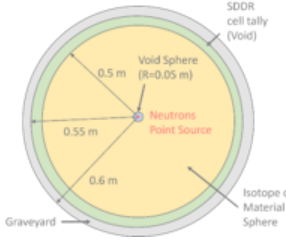


ASPIS Iron 88



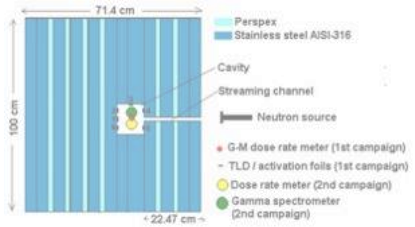
FNS W – BLKT -- TOF

ACTIVATION



Sphere SDDR

ITER CYL

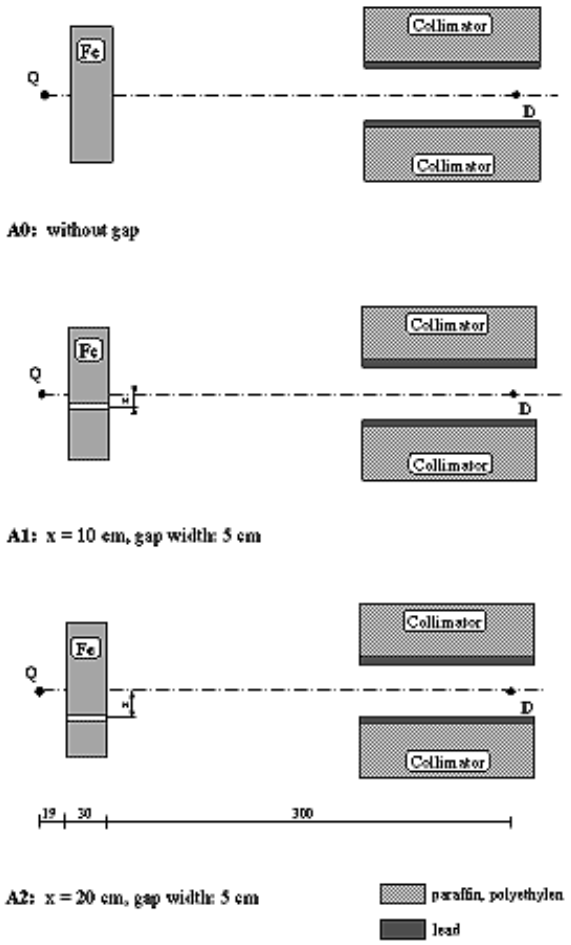


FNG SDDR

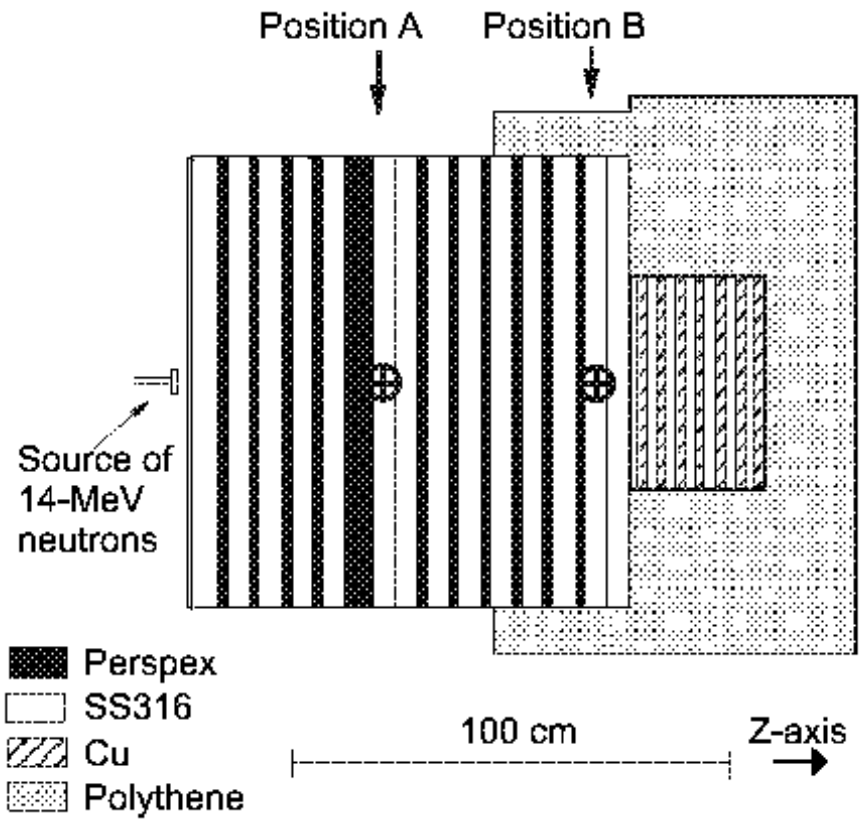
Iron results not in FENDL paper

14.1 MeV DT neutron source

TUD* iron slab



TUD* FNG bulk blanket



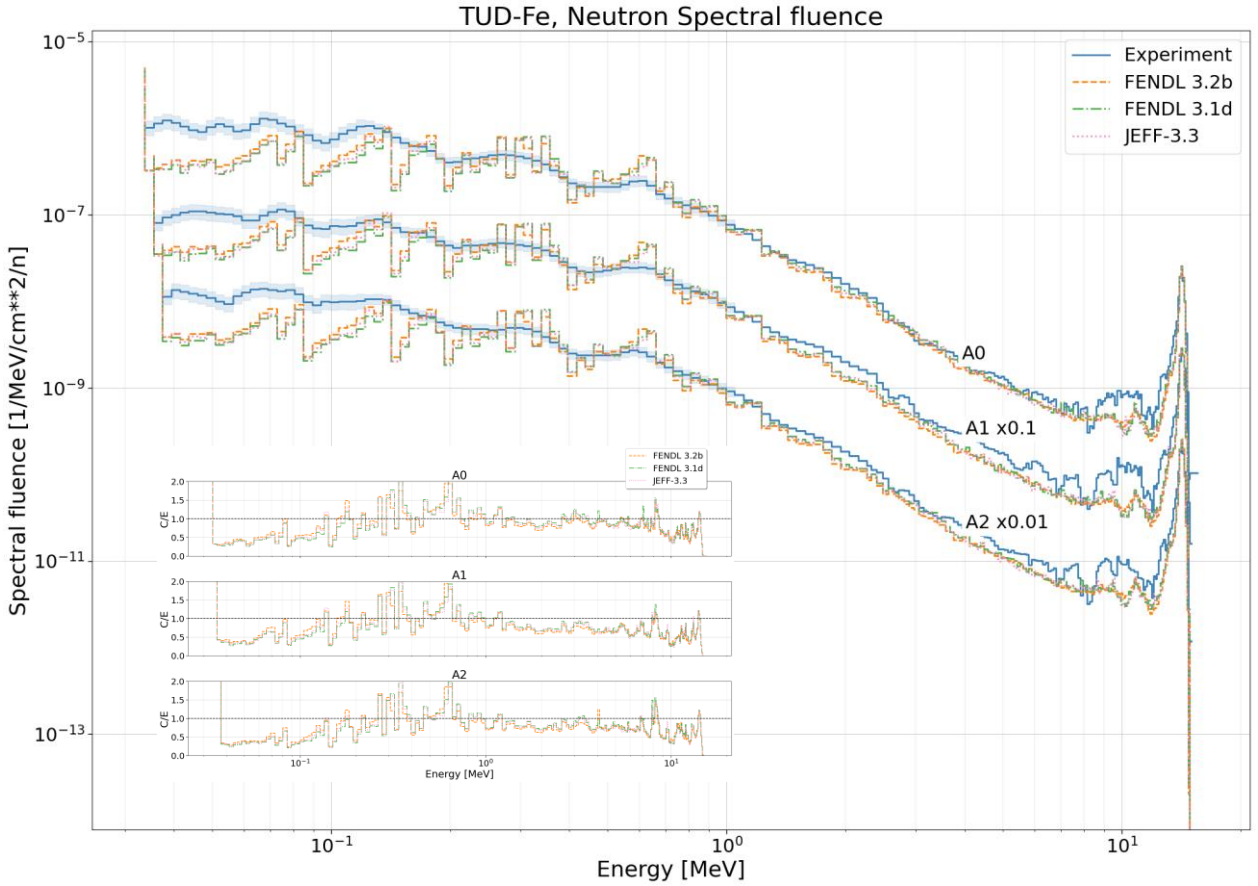
Position A: Measurement behind the 6 cm thick Perspex layer inside a SS316

Position B: Measurement in a SS316 layer at the total penetration depth

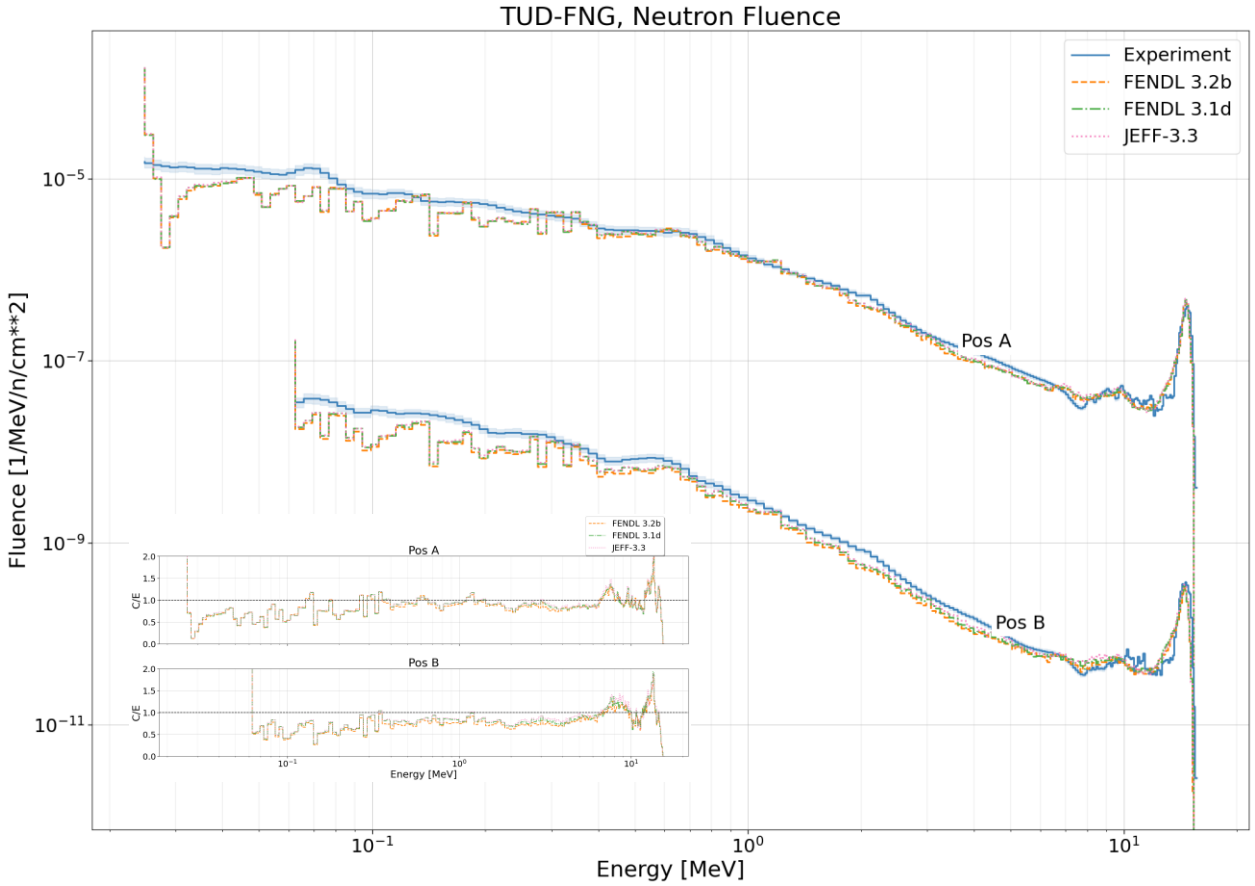
*Technische Universitaet Dresden

Neutron spectrum

TUD iron slab

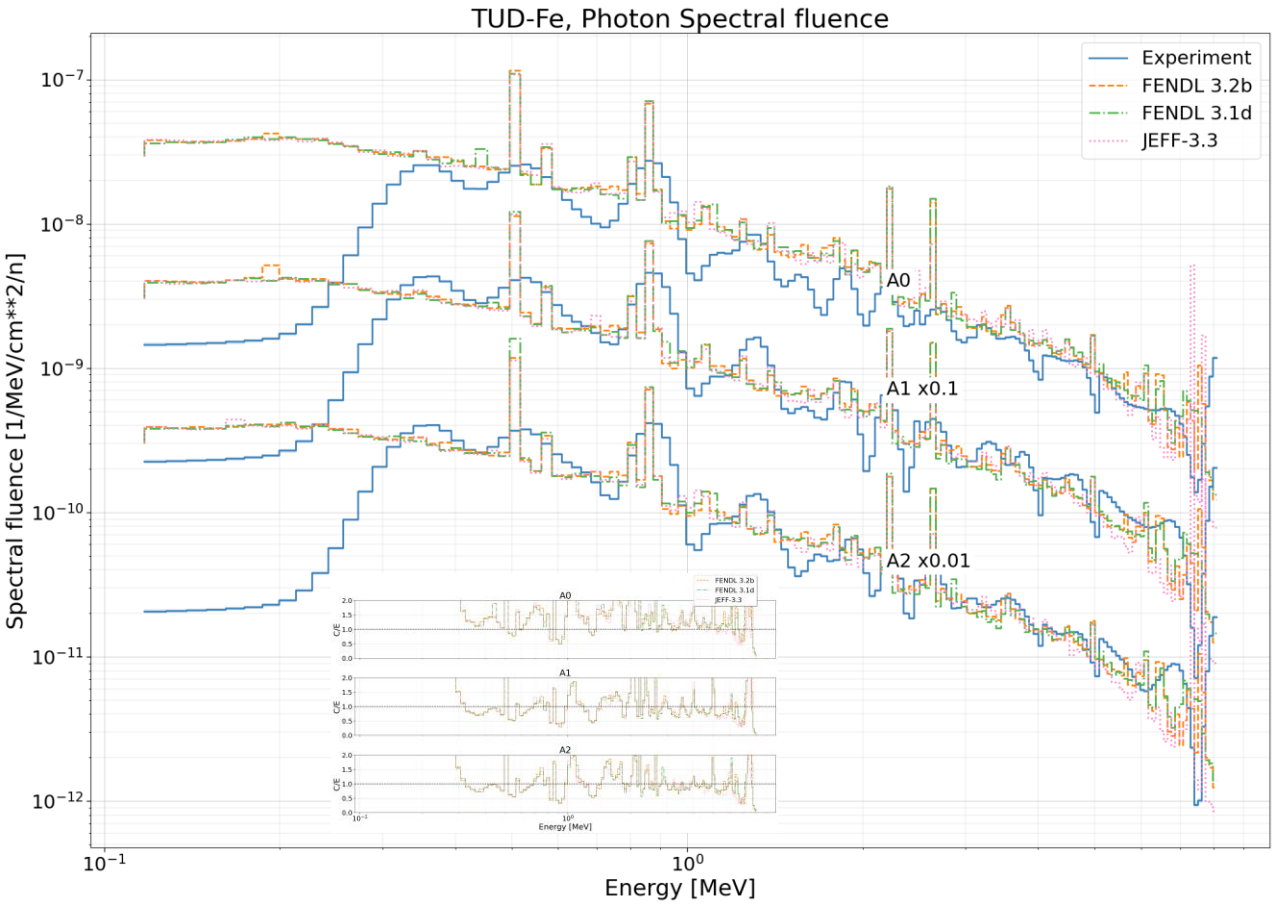


TUD FNG bulk blanket

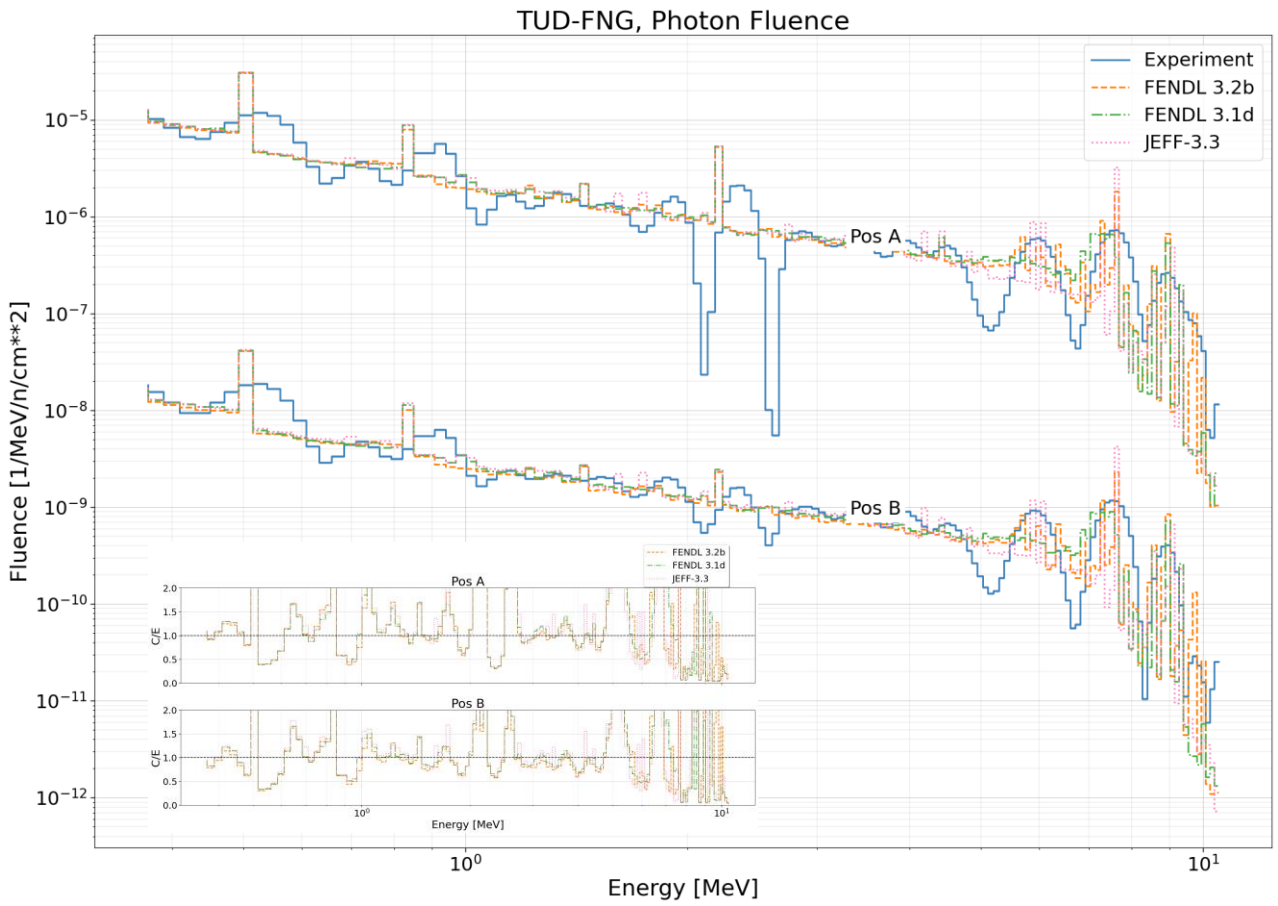


Photon spectrum

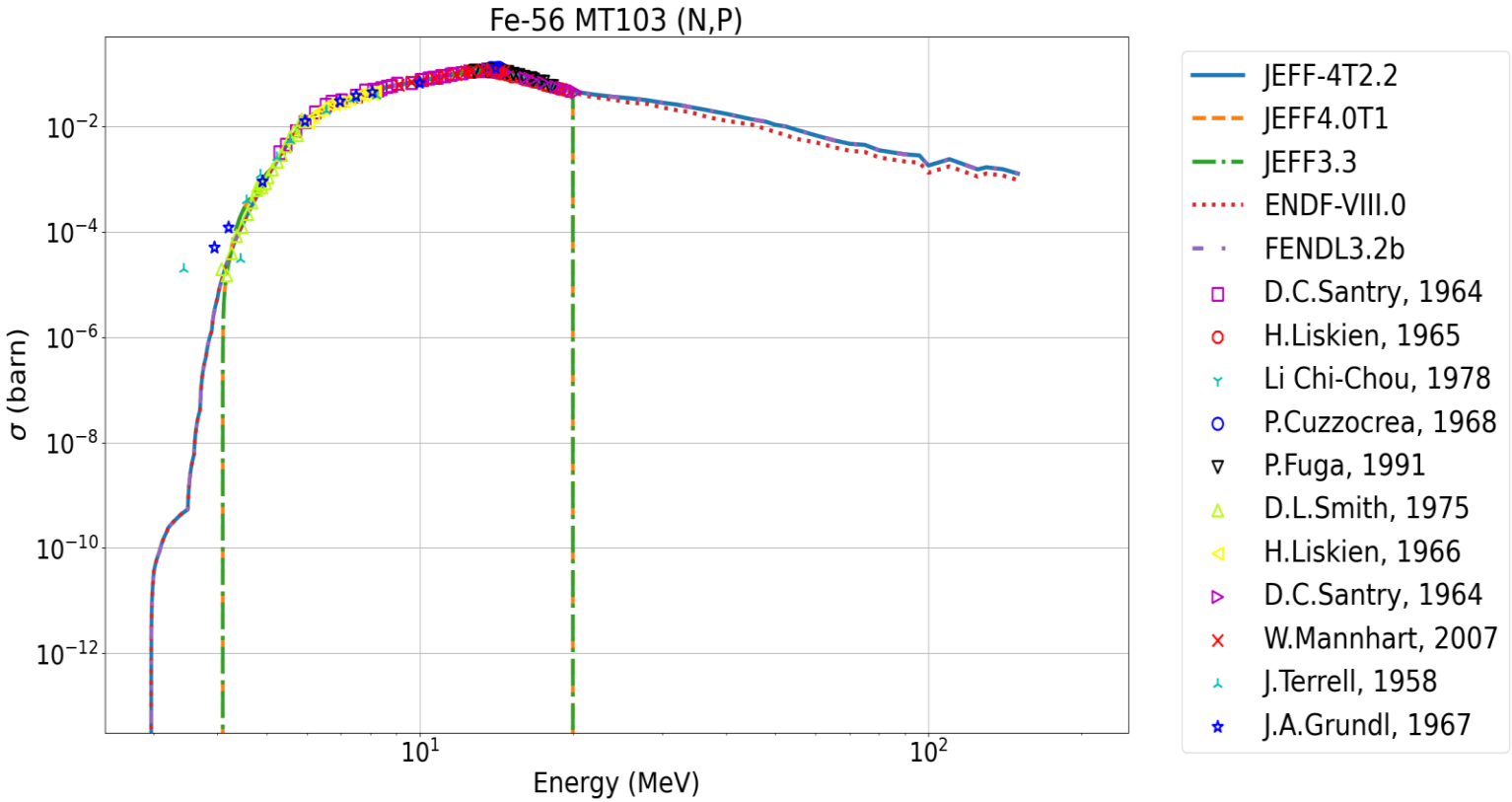
TUD iron slab



TUD FNG bulk blanket



New cross-sections plotter



Current features:

- Easy and quick **comparison between nuclear data libraries**
- Added the possibility of comparison with **EXFOR experimental data (requires optional ~1 GB package)**
- Implementation in JADE as **interactive** cross-section plotter (Linux branch)

Possible new features:

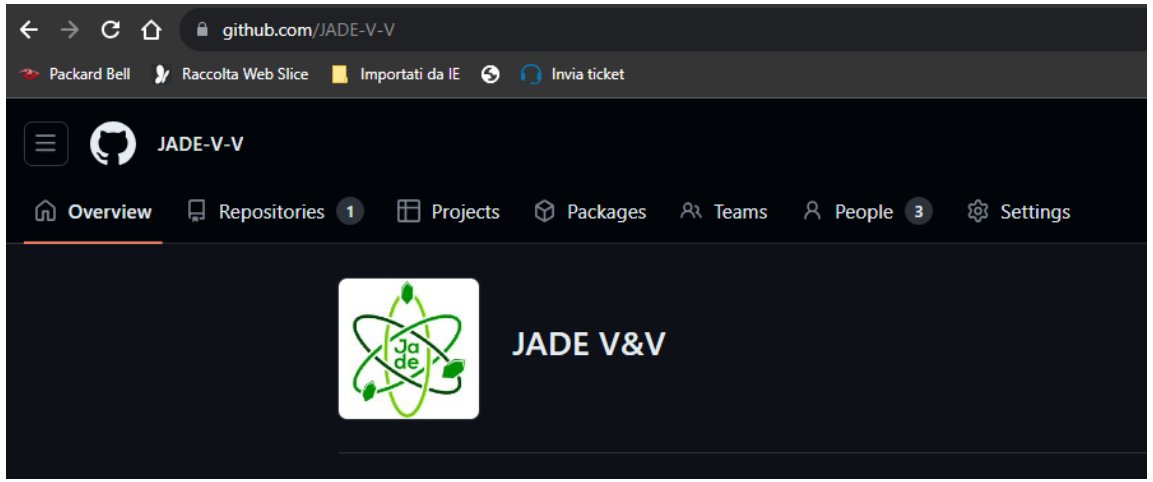
- Implementation of customizable ATLAS generation by means of a configuration file (on-going)
- Plot **materials' cross sections**

Transitioning to a more robust collective development project

JADE repository has been recently moved to the **JADE V&V organization.** This guarantees:

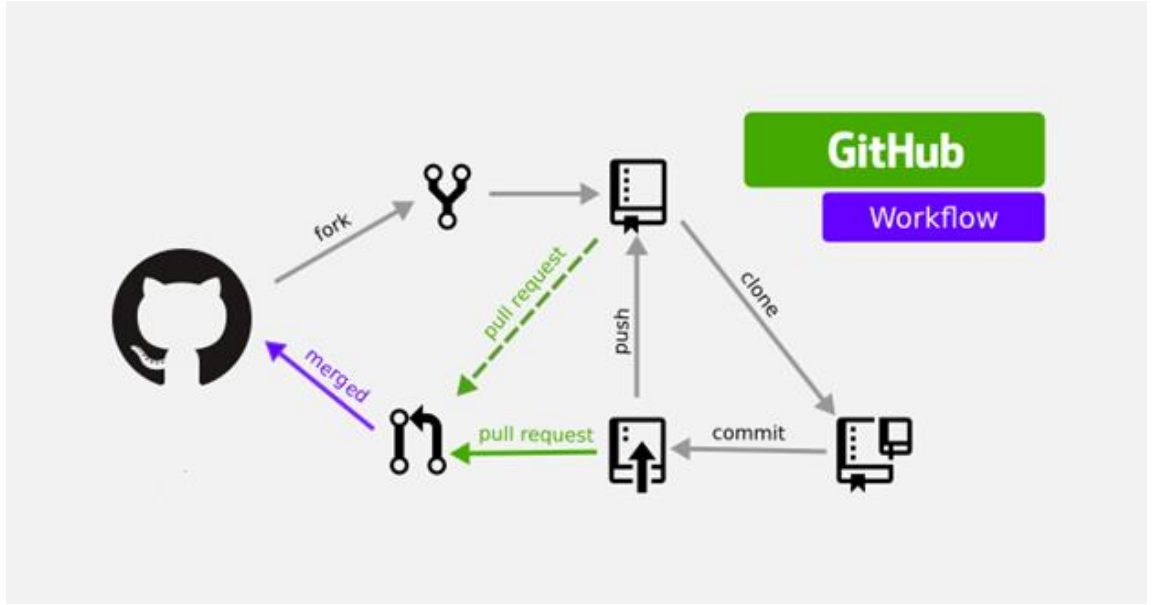
- Multiple owners
- Clearer setting of roles and rights from members and collaborators

https://github.com/JADE-V-V/JADE

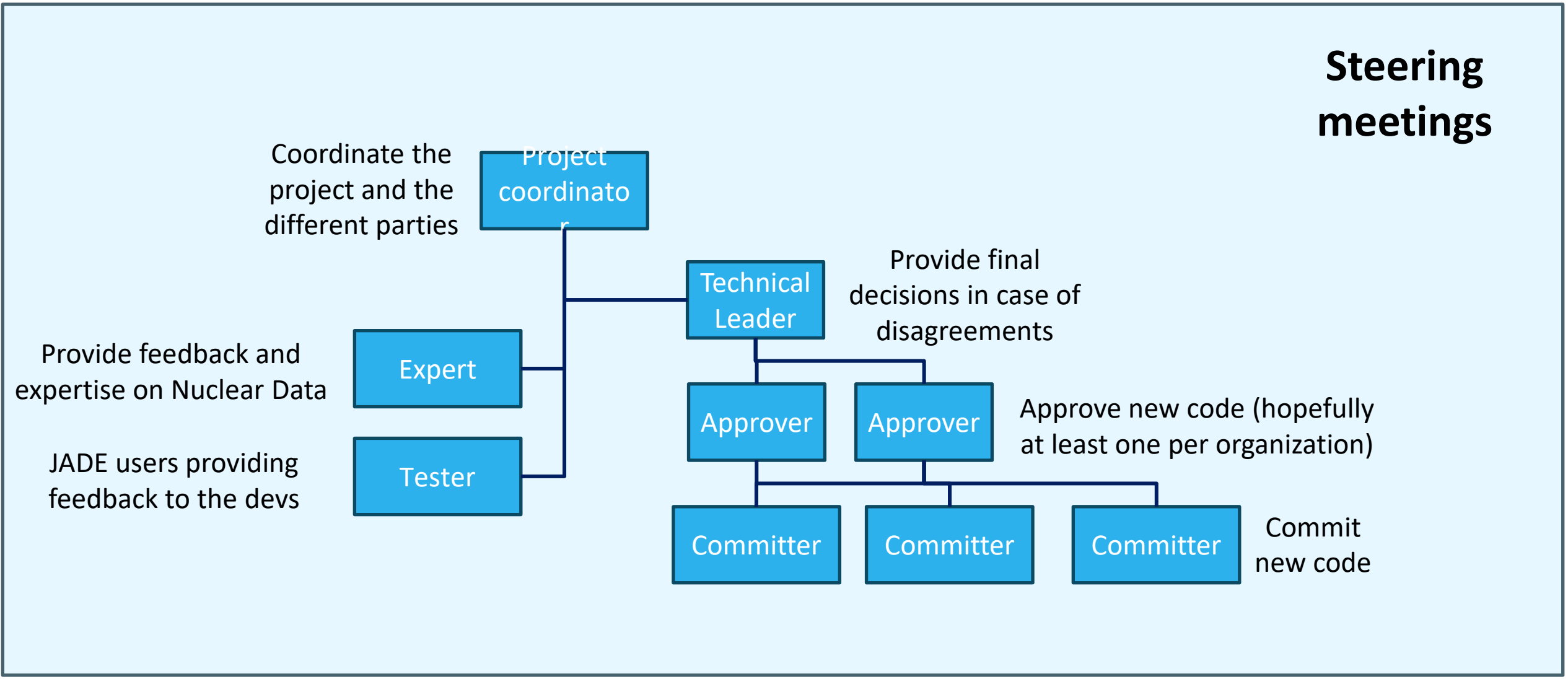


Contribution workflow based on fork and pull request to be merged to the developing branch after review from one of the authorized members.

Recognition of the different parties contributions.



Current JADE project structure



Roadmap

Jan/Feb 2024

Release of JADE v3.0.0*

Feb/March 2024

Steering meeting with all JADE stakeholders

Q4 2024

Beta of Serpent and OpenMC in JADE

Q4 2024

Inclusion of all FENDL3.2b benchmarks papers in JADE

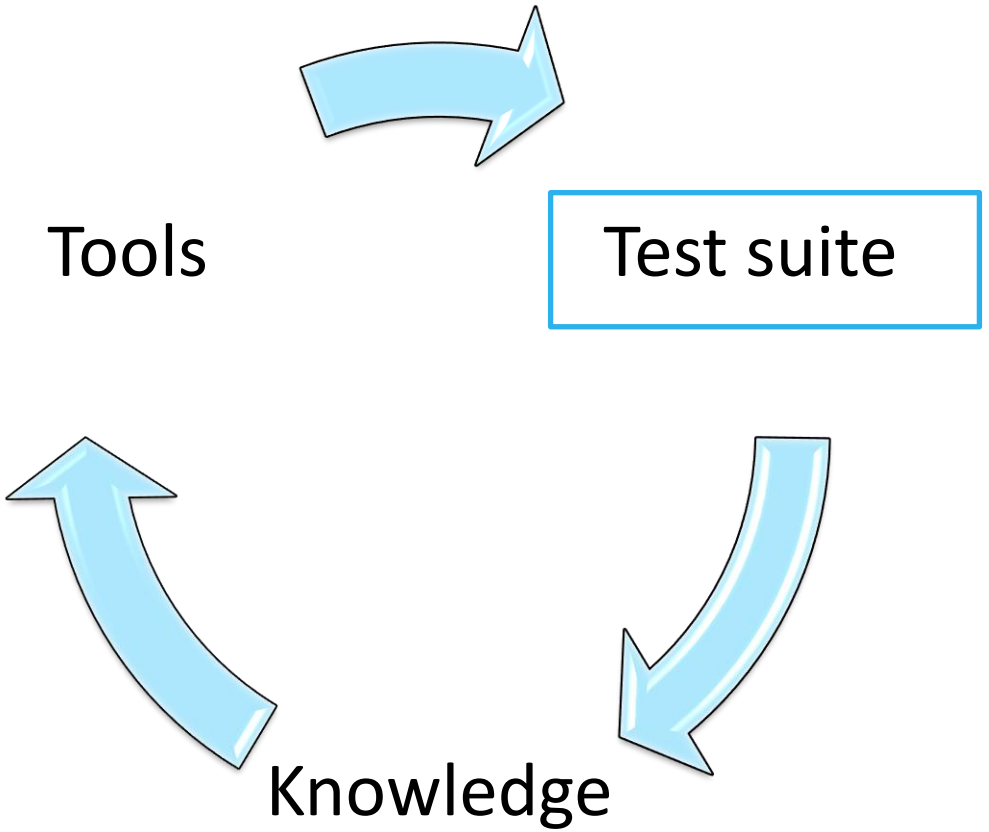
Q4 2025

Inclusion of benchmarks from JENDL papers

***JADE v3.0.0**: MCNP functionalities completely restored in Linux + preview of sphere for OpenMC and Serpent

Looking ahead

Looking ahead



Consolidation of all FENDL3.2 comp and exp benchmarks in JADE V&V tool suite

FUSION FOR ENERGY

Only ~50% of the FENDL3.2b paper are in JADE tool.

What we would like to avoid:

- Starting (almost) from scratch the next time we have to V&V a new FENDL release (e.g., see from FENDL2.1 case to FENDL3.2b)

What we foster:

- Usage of expert time on V&V case analysis and judgement, not on case preparation
- Progressive completion of V&V database and its standardization

What we propose:

- Recollection of latest MCNP inputs, post-processing routines and exp centralized by IAEA-NDS (e.g., this is usually asked also by journals).
- Insertion in JADE by the respective organization (F4E to coordinate/help/support).

Consolidation of all FENDL3.2 comp and exp benchmark in JADE V&V

Computational exercise

Computational benchmark/exercise	Made by	Implemented in JADE
Leakage Sphere	F4E	Yes
ITER 1-D	F4E	Yes
ITER 3-D	F4E	Yes
FNSF 3-D	UoW	No
FNSF 1-D	UoW	No
ITER-1D HCPB and WCLL TBM (F4E)	F4E	Yes
EU DEMO-3D divertor	Lituanian NA	No

Can be these already shared? Any foreseeable showstopper?

Consolidation of all FENDL3.2 comp and exp benchmark in JADE V&V

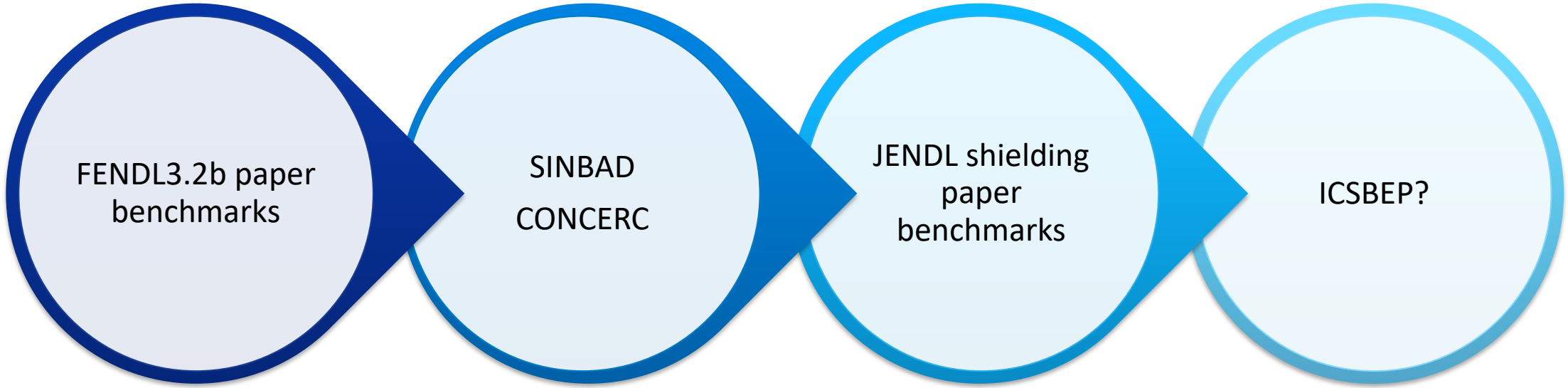
Experimental benchmark	Made by	Implemented in JADE
Oktavian	F4E	Yes
FNS experiments	JAEA	Partially
TIARA shielding experiments	JAEA	Yes
FNG Cu, WCLL, W-SS-Water shield	ENEA	Cu: No WCLL: No W-SS-Water:No
Research Center Rez 10.7 and 12.7 MeV quasi-monoenergetic neutron source: Dosimetrical reactions	CV Rez	No
Research Center Rez 252Cf(s.f.) source: Ni, Fe, Cu, stainless steel, and Pb leakage spectrum and dosimetrical reactions	CV Rez	No
LLNL Pulsed Sphere	Neudeker?	No
JET Activation Foils	JSI/UKAEA	No
SINBAD benchmarks: •ASPIS Iron 88 •PCA REPLICA •FNG SiC •FNG Tungsten •FNG HCPB •CIAE Fe	UKAEA	ASPIS Iron 88: Yes PCA REPLICA: No FNG SiC: No FNG Tungsten: Yes FNG HCPB: No CIAE Fe: No

Experimental benchmark

Implementation already on-going by UKAEA.

Looking forward

What's next on the tool suite implementation?

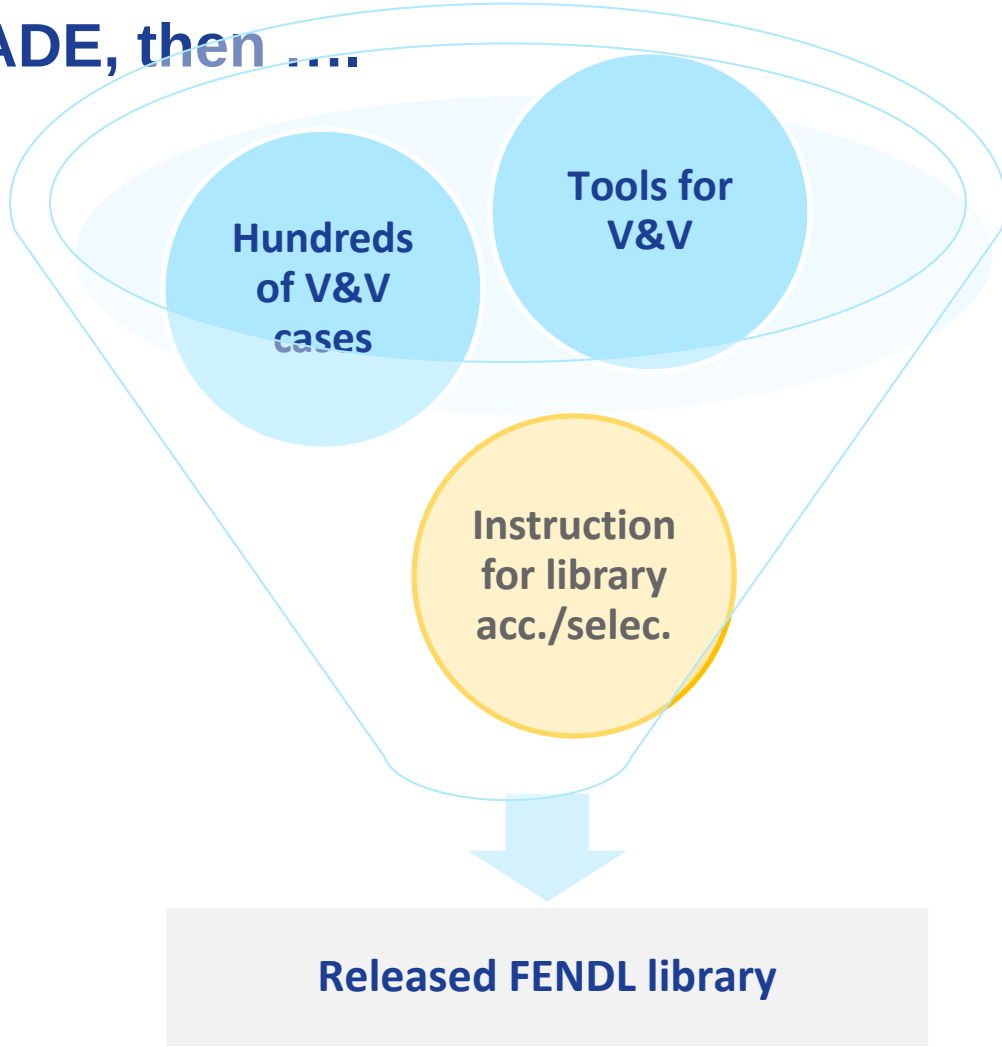


Looking forward

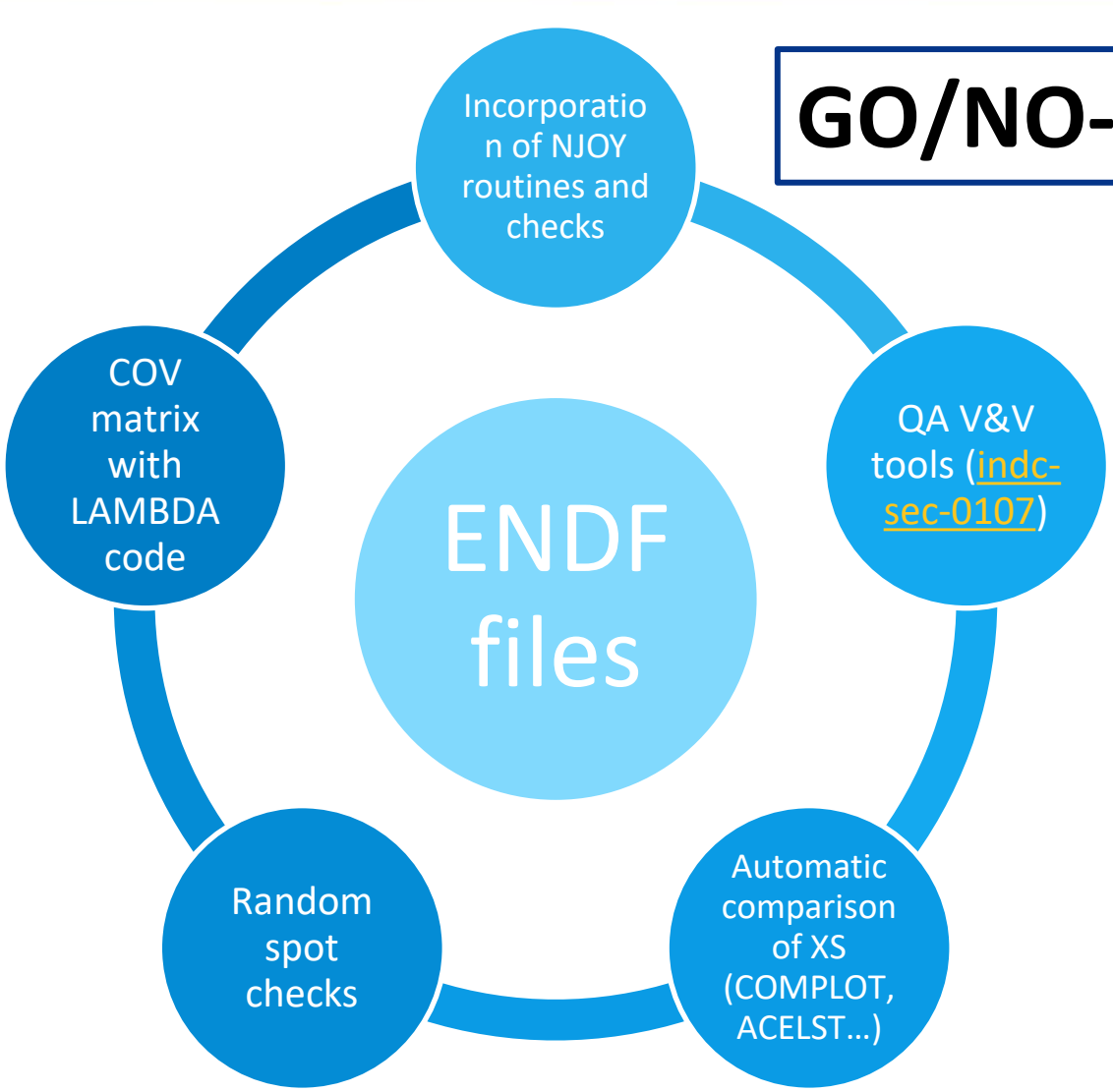
In few years we are going 50s of benchmark in JADE, then ….

How can we select the evaluation which overall performs better?

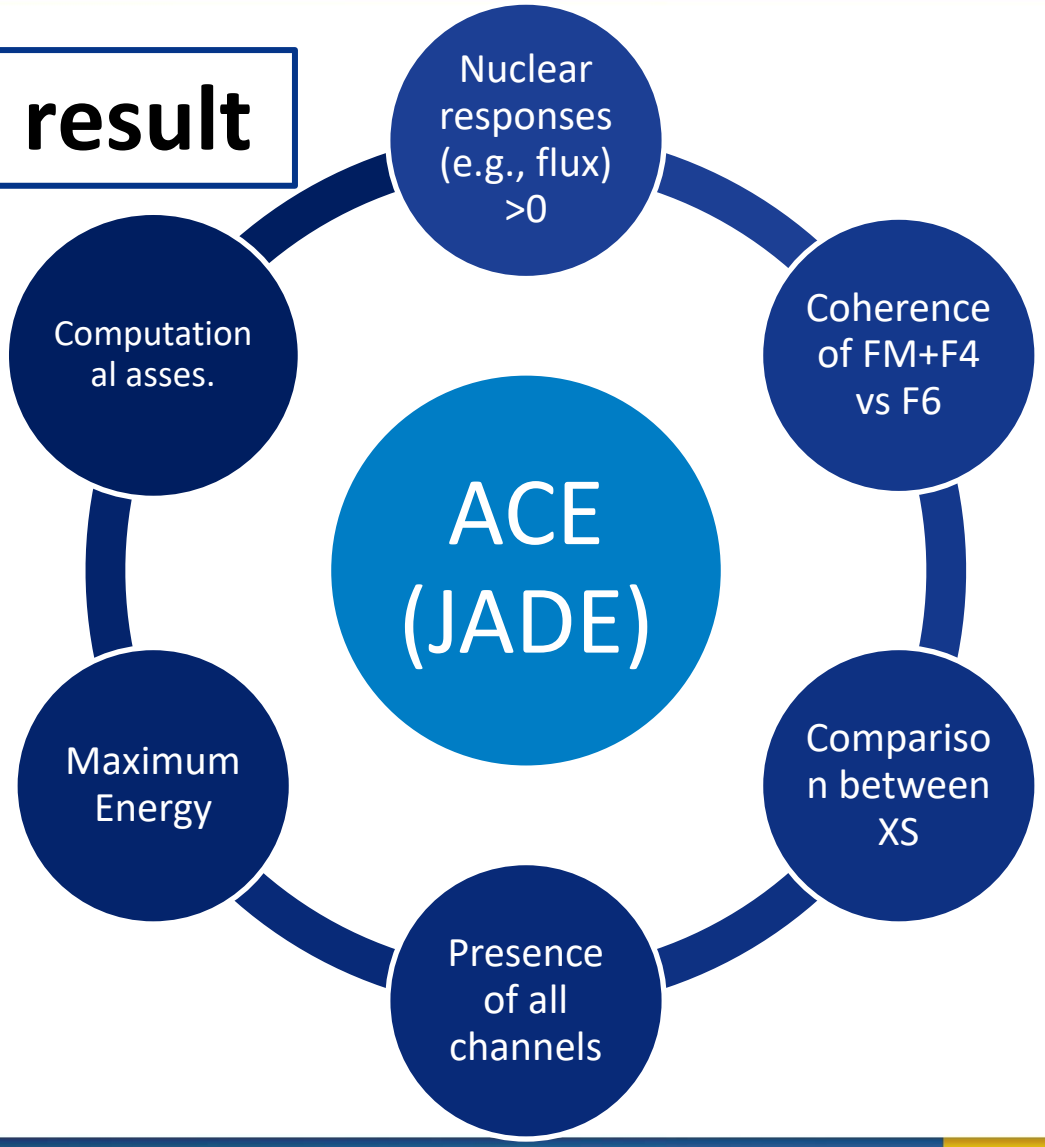
We still need instructions for the V&V of (fusion) libraries with clear acceptance/selection criteria (e.g., C/E TBR : [0.95, 1.05])



Very preliminary ideas for Verification: GO/NO-GO



GO/NO-GO result



Very preliminary ideas for Validation for FENDL (1/4)

We need to select the best evaluation for the FUSION application

Experimental databases

- SINBAD
- CONDERC
- ICSBEP
- …

Responses: C/E

- Flux
- Foils responses
- Heating
- …

Energy: C/E

- Very low
- Low
- Middle
- …

Fe

- TIARA
- ASPIS88
- FNS
- FNG
- Cf252
- …

How can we relate all these parameters together?

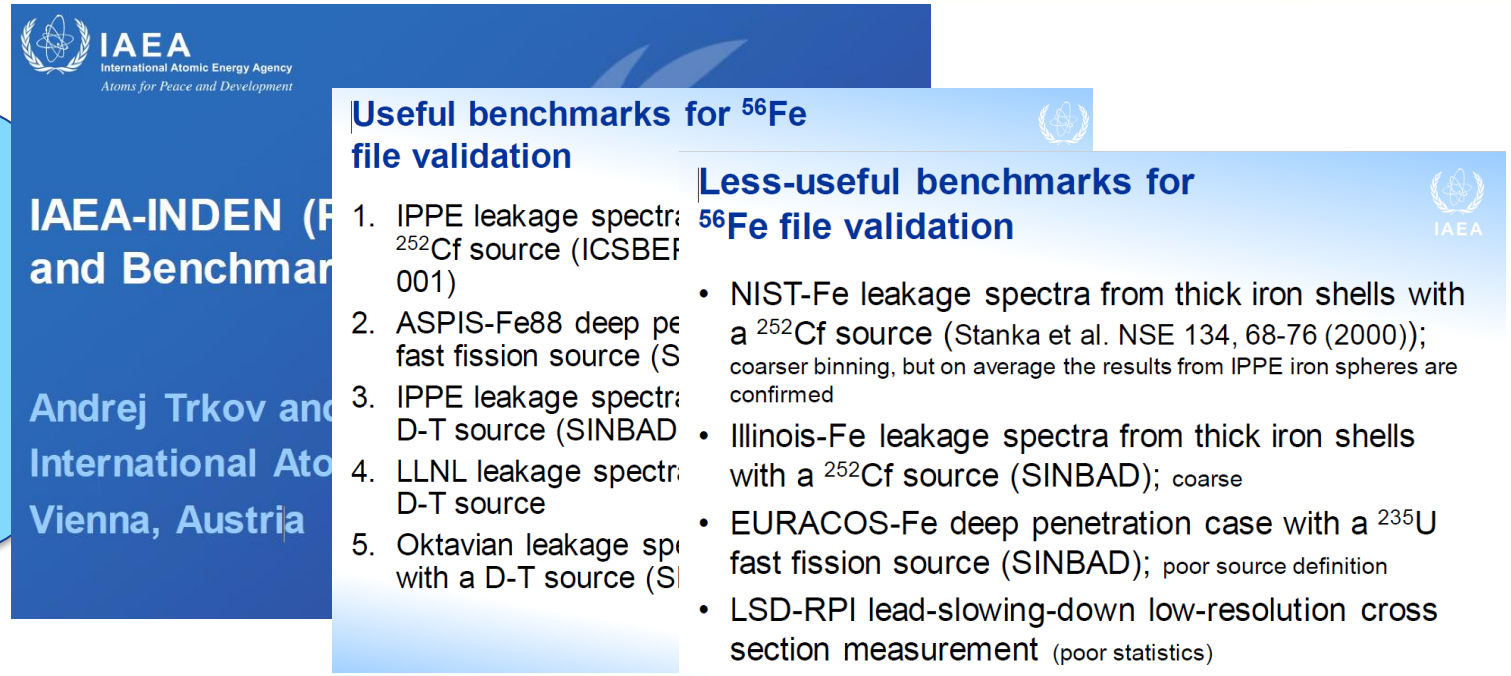
Rating/prioritizing the different parameters for fusion applications (e.g., 0-1, χ^2)!

Very preliminary ideas for Validation for FENDL (2/4)

FUSION FOR ENERGY

Experiment

- TIARA 40 Mev: 1.0
- TIARA 60 Mev: 0.6
- ASPIS88: …
- FNS: …
- …



Responses

- Flux: 1.0
- Foils: 0.8
- Heating: 0.6
- …

Energy: C/E relative importance

- Very low: 1
- Low: 0.8
- Middle: 0.6
- …

And what about C/E criteria?

Very preliminary Idea for Validation for FENDL (3/4)

And what about C/E? → χ^2 distribution

Development of the computational software tools to automate the computational analyses of fusion relevant benchmarks

S. Simakov, U. Fischer, A. Konobeyev

Karlsruhe Institute of Technology

To qualify the level of agreement we employed the standard metric for testing nuclear data libraries - the "reduced" chi-squared parameter:

$$\chi^2(n) = \frac{1}{n}\sum_{i=1}^{n}\frac{(C_i/E_i - 1)^2}{\sigma_i^2}$$

where the calculated and experimental values *Ci* and *Ei* for interval *i* are compared with unity mediated by the sum of the total MCNP simulation and experimental relative uncertainty σ_i. The degree of freedom, *n*, is considered to be equal to the number of Energy or TOF intervals (given in `Edges.dat`) in which the experimental and calculated neutron leakage spectra will be integrated. We also considered the partially cumulated $\chi^2(n)$ when the number of intervals *n* is lesser than maximal number necessary to cover the full Energy or TOF range of experimental data.

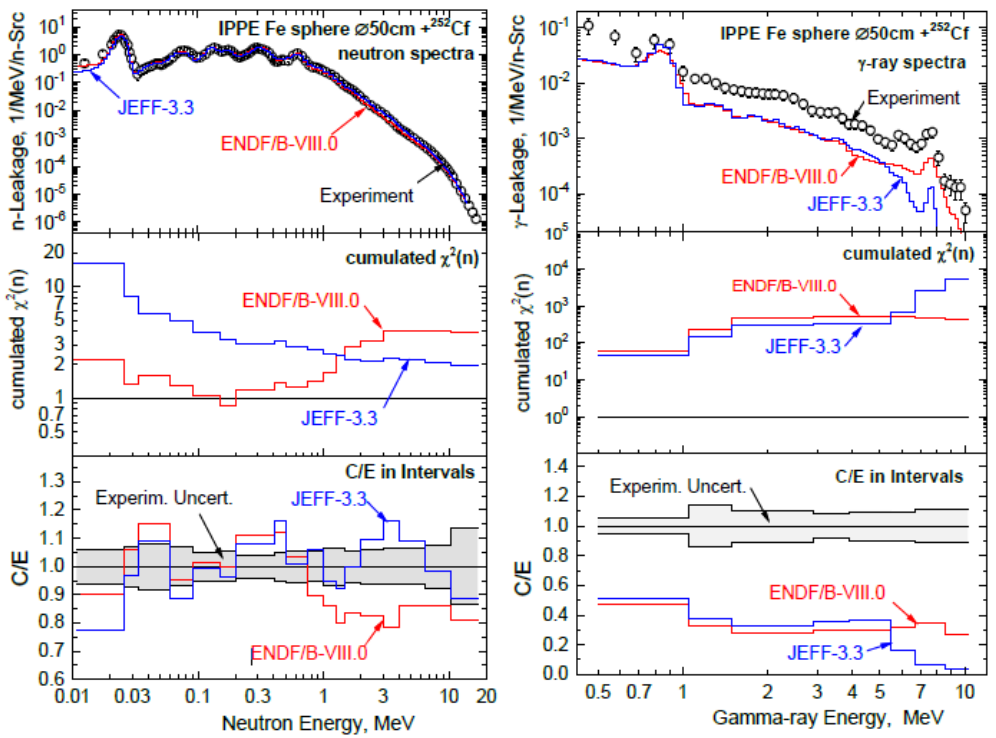


Fig. 5.1. The neutron (left) and γ-ray (right) leakage spectra from the IPPE iron sphere Ø50 cm with ^{252}Cf(s.f.) source: open circle - experiment [21, 23], curves - MCNP simulation with nuclear data from ENDF/B-VIII.0 (red) and JEFF-3.3 (blue). Upper part of figures – energy spectra, middle – χ^2 cumulated over *n* integration intervals, bottom – C/E for these intervals.

Very preliminary Idea for Validation for FENDL (4/4)

Experiment, w_V

- TIARA 40 Mev: 1.0
- TIARA 60 Mev: 0.6
- ASPIS88
- …

Responses, w_R

- Flux: 1.0
- Foils: 0.8
- Heating: 0.6
- …

Energy: C/E relative importance, w_K

- Very low: 1
- Low: 0.8
- Middle: 0.6
- …

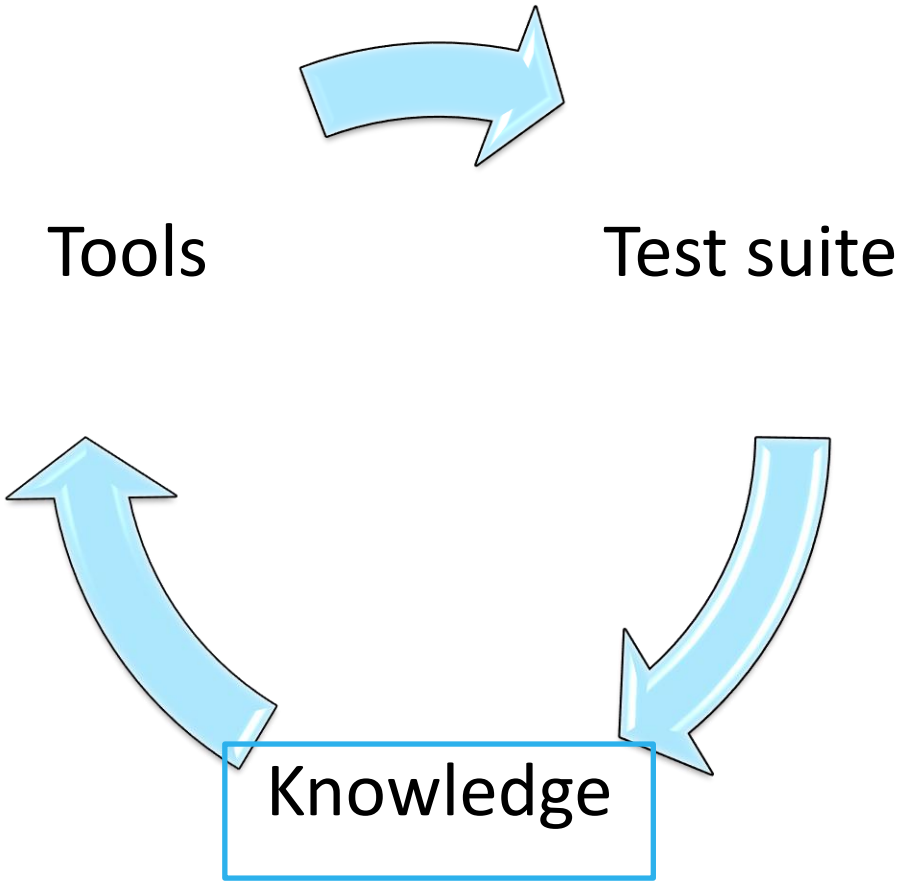
$$\chi^2(n) = \frac{1}{n} \sum_{i=1}^{n} \frac{(C_i/E_i - 1)^2}{\sigma_i^2}$$

$$Score_{LIBRARY_i} = \sum_{i=1}^{V} w_i \sum_{j=1}^{R} w_j \sum_{k=1}^{E} w_k \chi_{C,k}$$

$Score_{LIBRARY_i}\big|_{min}$ → **FENDL evaluation for the single channel/material**

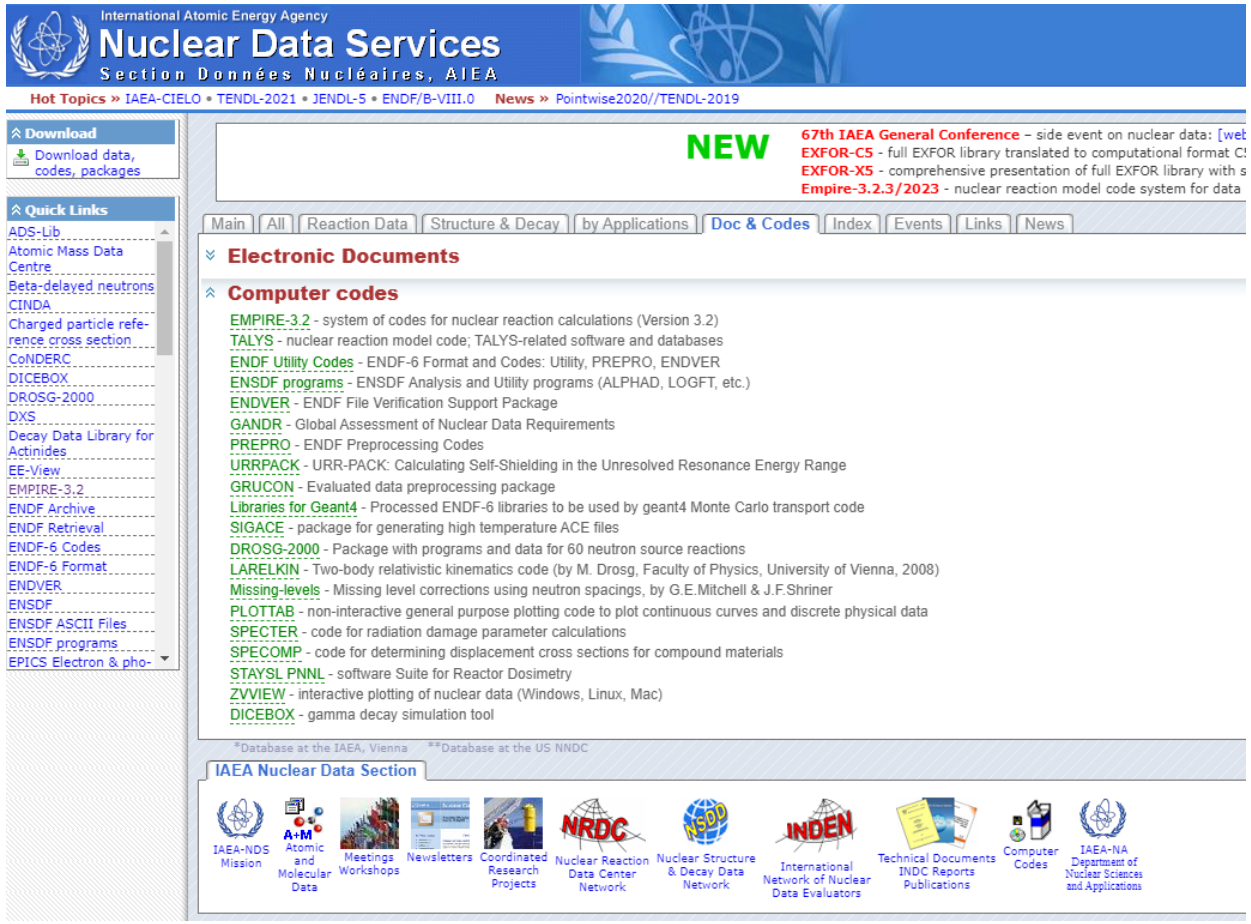
+ Expert JUDGEMENT

Looking ahead



Looking ahead

Addition of JADE to the IAEA Compute code list



This would allow to:

- Increase recognition from nuclear data word on the work carried so far.
- Possibly boost its visibility, usage and development.
- Endorse the F4E support on the activity for the short-medium term.

Looking ahead

Delivery of a formal letter from IAEA to ITER for the usage of FENDL3.2

IAEA

Atoms for Peace

الوكالة الدولية للطاقة الذرية
国际原子能机构
International Atomic Energy Agency
Agence internationale de l'énergie atomique
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Mr David Campbell

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2014-11-04

Dear Mr Campbell,

I am writing to inform you of recent work at the IAEA Nuclear Data Section of relevance to ITER. For many years the Fusion Evaluated Nuclear Data Library (FENDL) has been produced in various versions to meet the needs of Fusion Technology, in particular the ITER project. FENDL-2.1 is currently the reference set of nuclear data for ITER and is available for all ITER partners to use in design and safety calculations. In 2006 the International Nuclear Data Committee (INDC) recommended the extension of the FENDL library to cover proposed materials testing facilities. A Technical Meeting aiming at identifying possible detailed objectives for a CRP was held at IAEA, Vienna in 2007 leading to the approval of the CRP in December 2007. Following work in the three Research Coordination Meetings the FENDL-3 library was produced. Full details are available at the webpage https://www-nds.iaea.org/fendl30/ including links to documentation and library downloads. Since the production of the library in 2012 a process of validation was undertaken and in one of the reports, INDC(NDS)-0631 (Benchmarking of the FENDL-3 Neutron Cross Section Data Library for Fusion Applications, U. Fischer, M. Angelone, P. Batistoni, T. Bohm, K. Kondo, C. Konno, M. Sawan, R. Villari, B. Walker, March 2014) arrived at the conclusion that: "In general, FENDL-3, as compared to FENDL-2.1, shows an improved performance for fusion neutronics applications. It is thus recommended to ITER to replace FENDL-2.1 as reference data library for neutronics calculation by FENDL-3.0."

(Already done in precedence for FENDL3.0 recommendation, 2014)

Letter from IAEA on FENDL 3 (QDJ25M v1.0) (current)

Looking ahead

Generation on NEW MCNP-D1S using FENDL 3.2b (FENDL3.2b+TENDL-2017)

- In FENDL3.2b EAF-2007 activation data has been replaced by TENDL-17.
- Therefore, new D1S (Direct-one-step) ACE data needs to be reassembled to perform dedicated shutdown dose rate studies.
- This activity will be carried out under an F4E contract by UNED (G.Pedroche).
- Release of this library with dedicated V&V (as well as paper) is expected by Q3 2024.
- Moreover, dedicated activation studies already estimated the preliminary impact of the replacement of EAF-2007 activation by TENDL-17. Minimal impact for major radioactive elements expected.

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Nuclear data for D1SUNED for the study of ITER planned in-situ maintenance dose scenarios

G. Pedroche †, P. Sauvan †, J. Alguacil, J. Sanz, R. Juárez

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Looking ahead

The magic tables (on-going work)

Benchmark	Sub	JADE	CONDERC (1)	SINBAD (2)	JENDL-5 Pa
FNS Integral experiment (in-situ)	LiO2				
	Be				
	C			X	X
	Fe (+ secondary gammas)			X	X
	Cu			X	
	W (+ secondary gammas)			X	X
	SS316				
	Vanadium (+ secondary gammas)			X	
	LiAlO2 (+ secondary gammas)		X		
	Li2AlO3				
	Li2ZrO3 (+ secondary gammas)		X		
	Li2TiO3 (+ secondary gammas)		X		
	SiC				
	Hg (+ secondary gammas)				
	Ti + LiO2				X
	Mo + LiO2				X
	W + LiO2		X		
	Cu + LiO2				X
	Pb + LiO2				X
	Vanadium + LiO2				
	Line source and annular blanket				
	Fusion blanket				

Table 2 Summary of benchmarks and aspects covered

	FNG				Oktavian					FNS		
Material	ITER blanket mock-up	HCPB TBM mock-up	W block	ITER inboard shield mock-up with TFC	Fe	Ni	Al	W	Mn	W cyl.	Sphere leakage	Fe block with dog-leg
TBM functional materials		x										
Steel	x	x		x								
Fe					x							x
Ni						x						
Al							x					
W			x					x		x		
Mn									x			
Li, LiPb											x	
Be											x	
Measured												
n/g flux	x	x	x	x	x	x	x	x	x	x	x	x
nuclear heating			x	x								
SDDR	x											
T prod.		x										
Important												
Bulk shielding	x	x	x	x	x	x	x	x	x	x	x	x
Streaming	x											x

Conclusions

- A long standing effort by F4E has been carried out in the last 5 year to kick-off the JADE V&V tool suite which is now become of the cornerstone of the nuclear data V&V not only for FENDL but also for JEFF.
- F4E is willing to continue to coordinate and contribute to this effort in the benefit of all the nuclear data community. Stronger together.
- We acknowledge the support of many institutions (e.g., UKAEA, IAEA,…) for their contributions and guidance (e.g., see documentation and papers).
- We look forward to the IAEA-NSD support:
  - To recollect the benchmarks carried out within the FENDL3.2b V&V published exercise
  - To check the possibility to include JADE in the IAEA-NDS computer code lists
  - To communicate the officiality of FENDL3.2 to ITER by a formal letter
- We very welcome the effort of the IAEA-NSD to maintain alive the FENDL community and expert group activity.
- We kindly encourage the FENDL Expert consultant committee to start discussing the “instruction for V&V and acceptance of the FENDL libraries”.
- And if we have time…

Points for further discussion

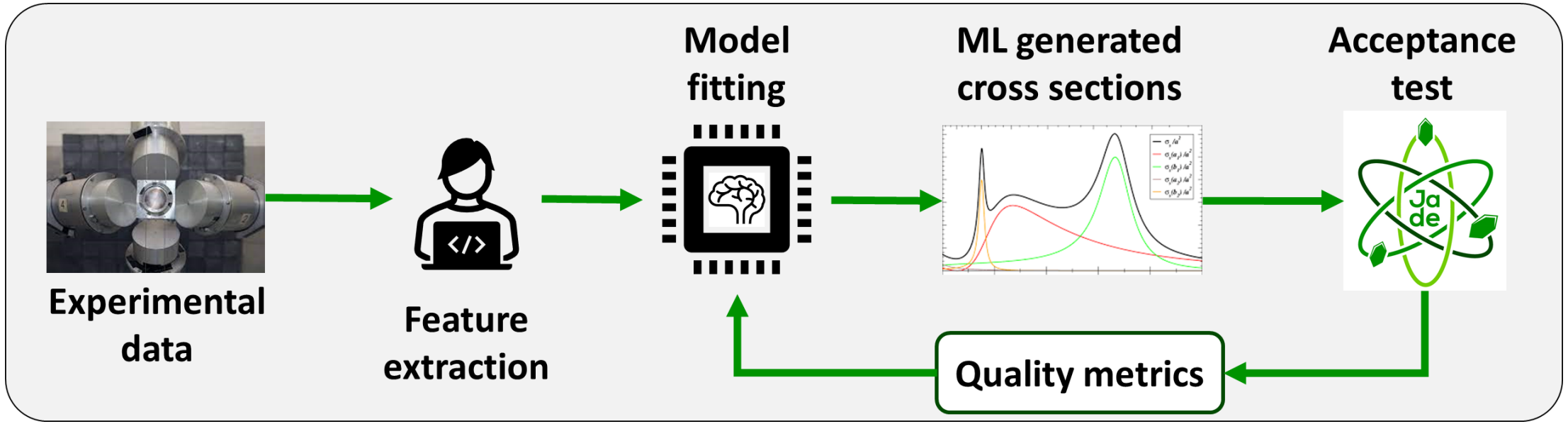
- Frequency of FENDL expert consultant meeting: one long in-person, one shorter remote?
- Plans for FENDL4.0 (and its relation with TENDL)
- How to better improve the communication via the expert group (e.g., bugs, proposal, collaborations…)
- FENDL toward a JEFF Gitlab model: generation, ENDF→ACE, testing...
- Usage of ML/AI in the improvement of nuclear data (see next)
- Issues of several benchmarks (e.g., missing data, error in MCNP models…)

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)

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