

Status of JADE and recent developments

Alberto Bittesnich, Davide Laghi*, Marco Fabbri*

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Outline



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



Quick refresh: What is Jade

Why JADE?



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

FENDL Quality Assurance: Proposal for V&V procedure

U. Fischer







What is JADE?







Continuous Integration









The Sphere Leakage benchmark is arguably the most important benchmark included in suite. Indeed, it allows to test individually each single isotope of the nuclear data librar assessment plus some typically used material in the ITER project namely:

At each push on the main JADE branch:

ITER CYLYNDER SDDF

[32%]

[44%]

[45%]

[63%]

[83%]

[88%]

[100%]

- 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







Recent advancements on F4E side

Benchmarks status





Iron results not in FENDL paper





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

Z-axis

*Technische Universitaet Dresden

Neutron spectrum

TUD iron slab



TUD FNG bulk blanket



Photon spectrum



TUD-Fe, Photon Spectral fluence TUD-FNG, Photon Fluence Experiment Experiment 10^{-7} FENDL 3.2b FENDL 3.2b FENDL 3.1d FENDL 3.1d 10^{-5} JEFF-3.3 JEFF-3.3 10-6 10^{-8} Spectral fluence [1/MeV/cm**2/n] Fluence [1/MeV/n/cm**2] 10^{-7} 10-8 10^{-9} FENDL 3.2b FENDL 3.1d JEFF-3.3 10^{-10} 10^{-11} 0.5 10-11 1.5 0.5 1.5 51.0-10-12 10-12 0.5 10° Energy [MeV] Energy [MeV] 10^{-1} 100 100 101 Energy [MeV] Energy [MeV]

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



FUSION

ENERGY

FOR

Roadmap





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









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	Νο

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		Evn
Oktavian	F4E	Yes		Ехр
FNS experiments	JAEA	Partially		ben
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	UKAEA	ASPIS Iron 88: Yes PCA REPLICA: No FNG SiC: No FNG Tungsten: Yes FNG HCPB: No CIAE Fe: No		lmp UKA
•CIAE Fe			_	

Experimental benchmark

Implementation already on-going by UKAEA.





What's next on the tool suite implementation?







Very preliminary ideas for Verification: GO/NO-GO





Footer (e.g. date, name of speaker, name of presentation...)





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



Experiment	IAEA International Atomic Energy Agency Atoms for Peace and Development	11	
 TIARA 40 Mev: 1.0 TIARA 60 Mev: 0.6 ASPIS88: FNS: 	IAEA-INDEN (F and Benchmar Andrej Trkov and International Ato Vienna, Austria	 IPPE leakage spectra ²⁵²Cf source (ICSBEF 001) ASPIS-Fe88 deep pe fast fission source (S IPPE leakage spectra D-T source (SINBAD IIIir LLNL leakage spectra D-T source Oktavian leakage sp with a D-T source (SI 	s-useful benchmarks for
Responses	E	nergy: C/E relative i	importance
 Flux: 1.0 Foils: 0.8 Heating: 0 	0.6	Middle: 0.6	And what about C/E criteria?



And what about C/E? $\rightarrow \chi^2$ 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:



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.

Footer (e.g. date, name of speaker, name of presentation...)

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



Energy: C/E relative importance, w_{κ} **Experiment**, w_v Responses, W_R TIARA 40 Mev: 1.0 Flux: 1.0 Very low: 1 TIARA 60 Mev: 0.6 Foils: 0.8 Low: 0.8 \bullet \bullet Heating: 0.6 Middle: 0.6 ASPIS88 igodol \bullet \bullet



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

 $Score_{LIBRARY_i}\Big|_{min} \rightarrow FENDL$ evaluation for the single channel/material

+ Expert JUDGEMENT









Addition of JADE to the IAEA Compute code list

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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.



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

diams for Perace

قوغانة الشرية المطاقة الثرية التراكية (王) (王) (王) (王) (王) (王) International Moneil Energy Agency Agence Internationale de l'énergie adomíque Mexajiyespaçõese auroritoria or a roomot segreme Mexajiyespaçõese auroritoria or a roomot segreme Organismo Internacional de Energia Adômica

Dial directly to extension: (+431) 2600- 21709

Mr David Campbell

Director for Plasma Operation Route de Vinon-sur-Verdon CS 90 046 13067 ST, PAUL-LEZ-DURANCE FRANCE Vienne International Centre, PO Box 100, 1400 Vienna, Austria Phone: (+43-1) 2600 + Fax: (+43-1) 26007 Email: Official Mail@isea.cog + Internet: http://www.isea.org. In redy please refer to:

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)



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.



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

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FNS

Table 2 Summary of benchmarks and aspects covered

Oktavian

FNG

				SINBAD (2 💌	JENDL-5 Paj		ITER blanket mock- up	HCPB TBM mock- up	W block	shield mock-	Fe	Ni	AI	w	Mn	W cyl.	Sphere leakage	with dog-
	LiO2 Be					Material				up with TFC								leg
	C			X	х	wateria				IFC								
	Fe (+ secondary gammas)			X	X	TBM												
	Cu			X		functional		x										
	W (+ secondary gammas)			X	X	materials												
	SS316					Steel	x	x		x								
	Vanadium (+ secondary gammas)			X		Fe					~							~
	LiAlO2 (+ secondary gammas)		x								x							x
						Ni						X						
	Li2AlO3					Al							x					
NS Integral experiment (in-situ)	Li2ZrO3 (+ secondary gammas)		X			w			x					x		x		
nas integral experiment (in-situ)	Li2TiO3 (+ secondary gammas)		x			Mn									x			
	SiC					Li, LiPb											x	
	Hg (+ secondary gammas)					Be											x	
	Ti + LiO2				X												^	
	Mo + LiO2				X	Measured												
	W + LiO2		x			n/g flux	x	x	x	x	x	x	x	x	x	x	x	x
	Cu + LiO2				x	nuclear			x	x								
	Pb + LiO2				X	heating			Â	î								
	Vanadium + LiO2					SDDR	x											
	Line source and annular blanket												-					
	Fusion blanket		I			T prod.		X										
		Important																
							x	x	x	x	x	x	x	x	x	x	x	x
						Streaming	x											x
						B												

Footer (e.g. date, name of speaker, name of presentation...)

The magic tables (on aging work)

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 \rightarrow 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 NucML¹: <u>https://pedrojrv.github.io/nucml/index.html</u>

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



Thank you for your attention

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