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PLATAFORMA TECNOLÓGICA DE ENERGÍA NUCLEAR DE FISIÓN

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Processing & Benchmarking JEFF-4T2.2 – A comparison with other evaluations

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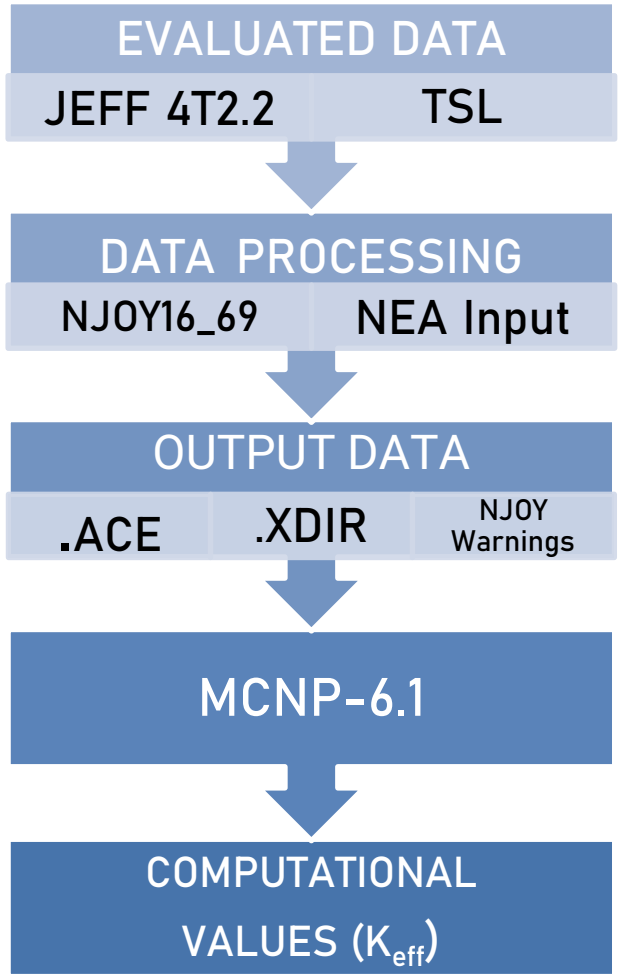
“Impact of recent nuclear data evaluations on energy and non-energy nuclear applications”

23/05/2023

Content

- Processing evaluated data from JEFF4-T2.2
  - Methodology and input files
  - Python code for processing ACE files
- Criticality Benchmarking – Mosteller's suite with 123 ICSBEP Benchmarks
  - Comparison NEA – UPM processing
  - Comparison benchmarking with other libraries
  - Sensitivity analysis
- Shielding Benchmarking
  - OKTAVIAN

Processing evaluated data from JEFF4T2



- Evaluated data from JEFF4-T2.2 (February 2023)
- ENDF (564 isotopes) and Thermal Scattering Laws materials.
- Processsing with NJOY2016 (v.69) using NEA Input parameters.
- For each .ENDF file processed we get:
  - .ACE file -> MCNP
  - .XDIR file -> MCNP
  - Warning Log -> Feedback
- Run Mosteller's Suite with MNCP-6.1 to get k-effective values of each experiment.

```
moder / Convert data
20 -21
reconr / Reconstruct XS for neutrons
-21 -22
'pendf for material ngeniso'/
ngeniso/
0.001/
0/
moder
-22 42
broadr / Doppler broaden neutron xs
-21 -22 -23
ngeniso 1/
0.001/
293.6/
0/
thermr
0 -23 -24
0 ngeniso 20 1 1 0 0 1 221 0/
293.6/
0.001 10/
moder
-24 44
purr / Process Unresolved Resonance Range
-21 -24 -25
ngeniso 1 1 20 64/
293.6/
1.e+10/
0 /
acer / Prepare ACE files
-21 -25 0 32 33/
1 1 1 0.40 0/
'Ace for ngeniso'
ngeniso 293.6
1 1/
/
acer
0 32 34 38 39/
7 1 1 -1/
'Ace for ngeniso - check 1'/
viewr
34 48/
moder
-23 36
stop
```

Figure 1. NJOY Input to generate ACE files

Processing evaluated data from JEFF4T2

```
#Lectura de la lista de isotopos
isotopos=os.listdir('Lib')
nisotopos=len(isotopos)
for i in range(0,3):
    start=time.time()
    nomarchivo=isotopos[i][:-4]
    filedir="Lib/"+isotopos[i]
    with open(filedir, 'r') as file:
        data = file.readlines()
        nmat=data[2][66:70]
#################################################################
    origen="Lib/" + isotopos[i]
    shutil.copy(origen, 'tape20')
#################################################################
#Edicion input
    shutil.copy('GenericInput.INP', 'Input.INP')
    search_text = "ngeniso"
    replace_text = str(nmat)
    with open(r'Input.INP', 'r') as file:
        data = file.read()
        data = data.replace(search_text, replace_text)
    with open(r'Input.INP', 'w') as file:
        file.write(data)
#################################################################
#Llamada a .bat generico
    subprocess.call('procesa.bat')
    os.remove('Input.INP')
    print(nomarchivo,'processed.',)
#################################################################
#Se renombran los archvios
    salidaace="Outputs/ACE/"+ nomarchivo +".ace"
    shutil.copy('generic.ace', salidaace)
    os.remove('generic.ace')
#################################################################
    salidaxsdir="Outputs/XSDIR/"+ nomarchivo +".XSDIR"
    shutil.copy('generic.XSDIR', salidaxsdir)
    os.remove('generic.XSDIR')
    search_text = "filename route"
    replace_text = nomarchivo +".ace"+" 0"
    with open(salidaxsdir, 'r') as file:
        data = file.read()
        data = data.replace(search_text, replace_text)
    with open(salidaxsdir, 'w') as file:
        file.write(data)
#################################################################
    salidaps="Outputs/Otros/"+ nomarchivo +".ps"
    shutil.copy('generic.ps', salidaps)
    os.remove('generic.ps')
    salidapendf="Outputs/Otros/"+ nomarchivo + ".pendf"
    shutil.copy('generic.pendf', salidapendf)
    os.remove('generic.pendf')
    salidaout="Outputs/Otros/"+ nomarchivo + ".out"
    shutil.copy('generic.out', salidaout)
os.remove('generic.out')
    finish=time.time()
    print('Processing time:',round((finish-start)/60,2),'minutes \n')
```

Figure 2. INGENIA Group Python code for ACE files processing.

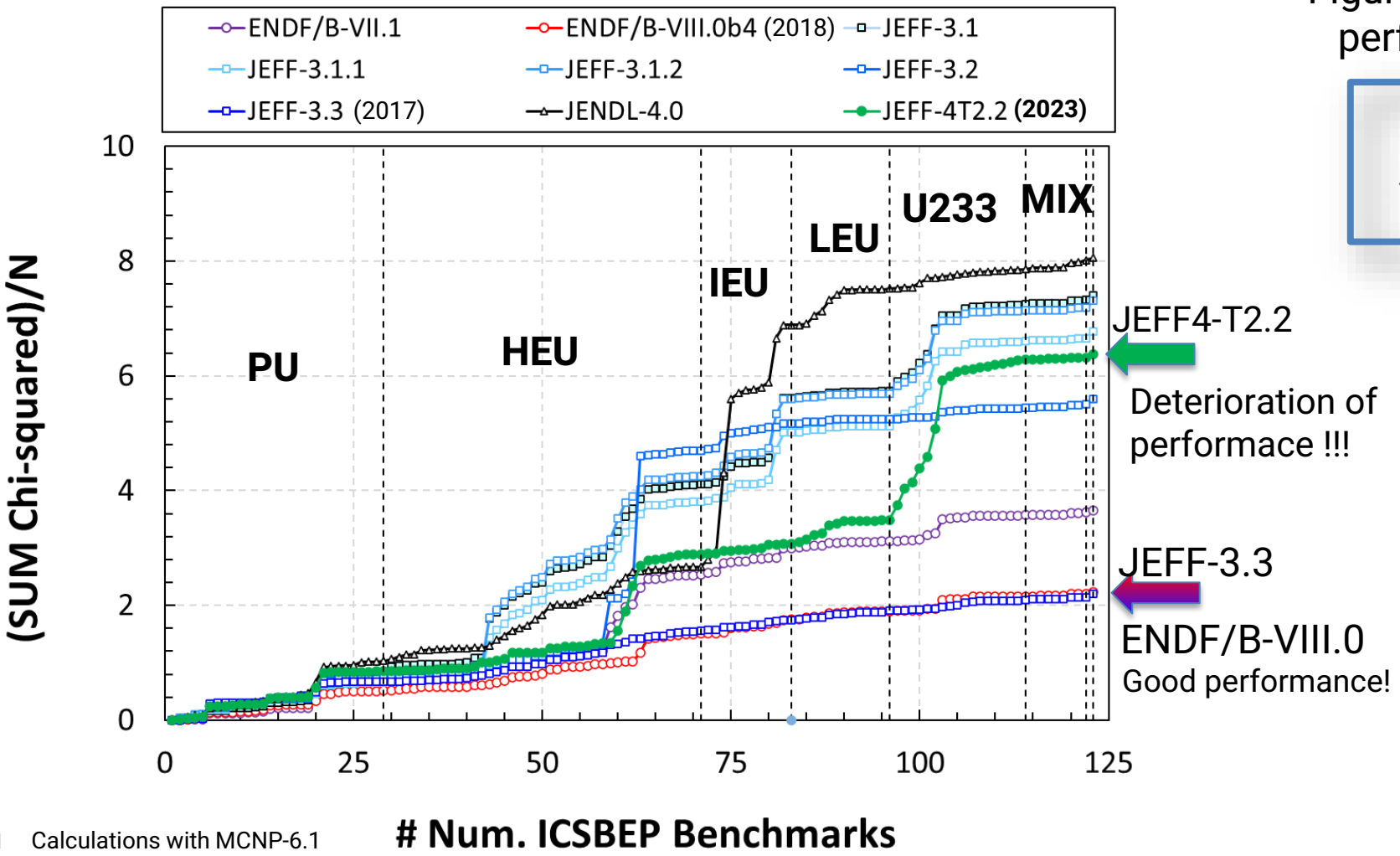
Figure 3. INGENIA Group Python code for warning logging.

```
with open(r'generic.out', 'r') as file:
        out = file.read()
        print('Number of warnings:', out.count('message'))
    a=0
    b=0
    c=0
    module=0
    if os.path.isfile('Outputs/WarningLog.xlsx'):
        aviso=pd.read_excel('Outputs/WarningLog.xlsx')
    else:
        aviso=pd.DataFrame()
        aviso['Date']= None
        aviso['Isotope']=None
        aviso['Module']=None
        aviso['Warning']=None

headend=out.find('****************************************
**********************************',out.find('***************
************************************************************
*')+1)
    while (module != -1):
        module=out.find('.', headend +80)
        modwarn=out[headend+80:module]
        a=out.find('message', module)

nxtheadend=out.find('****************************************
**********************************', module )
        while (a < nxtheadend) &  (a != -1):
            b=out.find('\n', a)
            c=out.find('\n',b+1)
            warn=out[a:c]
            line={'Date':time.strftime("%d/%m/%y
%H:%M:%S"),'Isotope':nomarchivo,'Module':modwarn.upper(),'War
ning':warn}
            aviso=aviso.append(line,ignore_index=True)
            a=out.find('message', c)
        headend=nxtheadend
    aviso.to_excel('Outputs/WarningLog.xlsx', index=False)
```

- INGENIA Team has created a Python code for processing .ACE and .XDIR files.
- The code automates the processing of all .ENDF files, avoiding having to process each file one by one.
- The code generates a log with all the warnings from NJOY.

Criticality Benchmarking – Mosteller's suite with 123 Benchmarks

Criticality Benchmarking: Mosteller's Suite - 123



JEFF4-T2.2

Deterioration of performace !!!

JEFF-3.3

ENDF/B-VIII.0
Good performance!

Figure of Merit to assess an overall performance of ND in criticality:

$$\chi^2 = \frac{1}{N} \cdot \sum_{i=1}^{N} \frac{\left(k_{C,i} - k_{E,i}\right)^2}{\Delta k_{C,i}^2 + \Delta k_{E,i}^2}$$

Table 1. Differences in keff using different ACE files UPM vs NEA (only cases > 10 pcm)

Δkeff (in pcm)	ICSBEP
19	MIX-COMP-THERM-002-005
17	U233-SOL-INTER-001-001
-13	HEU-MET-FAST-003-011
-19	MIX-COMP-THERM-002-001
-50	U233-COMP-THERM-001-003

- Calculations with MCNP-6.1

Criticality Benchmarking – Mosteller's suite with 123 Benchmarks

Criticality Benchmarking: Mosteller's Suite - 123

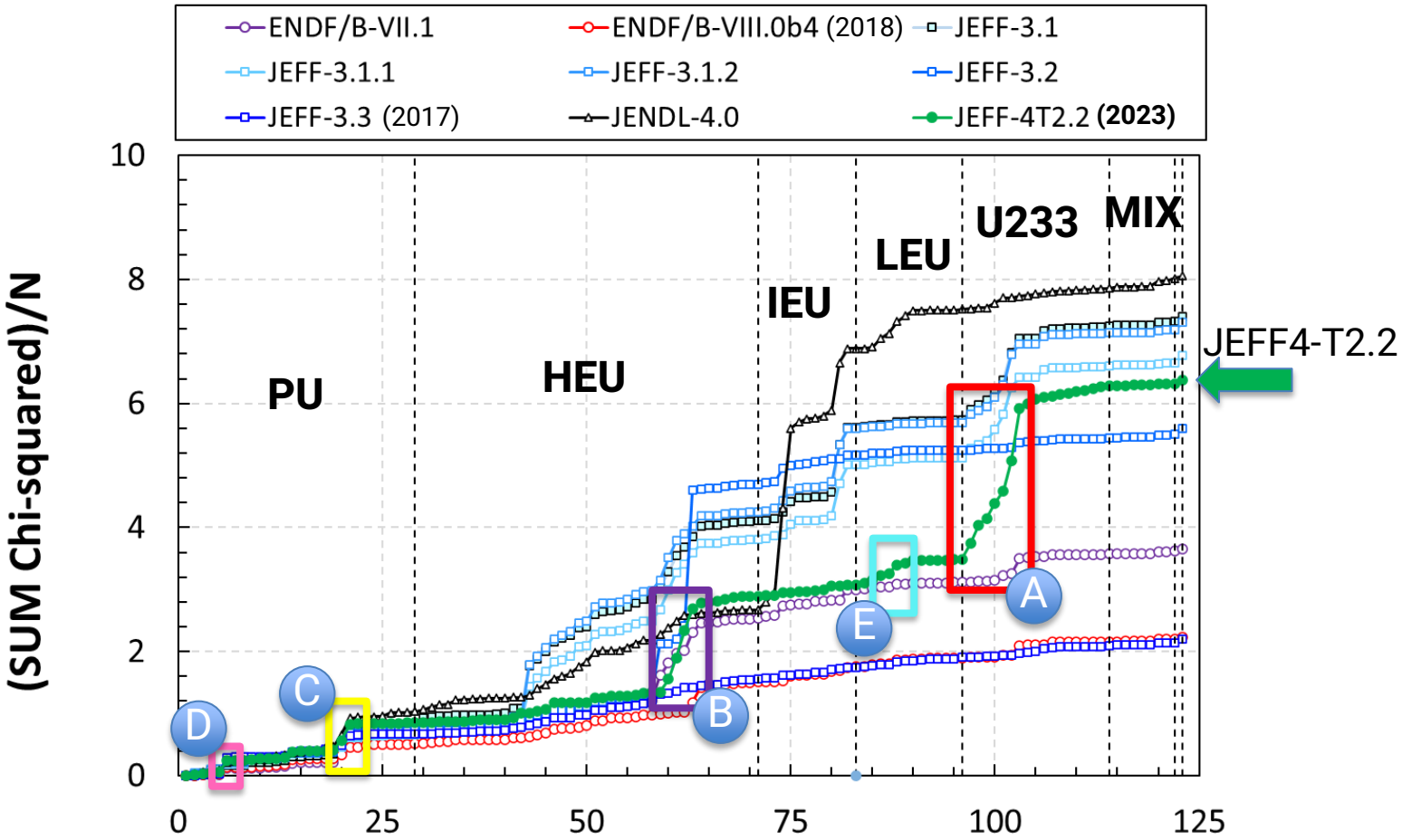


Table 2. Cases with highest Chi2 values

#Z	#ID	CASE	Chi2
A	103	U233-MET-FAST-004-002	**104.3**
A	102	U233-MET-FAST-004-001	**58.8**
B	62	HEU-MET-INTER-006-003	**54.3**
B	63	HEU-MET-INTER-006-004	**43.7**
B	61	HEU-MET-INTER-006-002	**42.8**
A	98	U233-MET-FAST-002-001	**36.3**
A	97	U233-MET-FAST-001-001	**31.3**
C	21	PU-SOL-THERM-009-003	**31.0**
A	100	U233-MET-FAST-003-001	**30.0**
B	60	HEU-MET-INTER-006-001	**25.0**
A	101	U233-MET-FAST-003-002	**24.7**
D	6	PU-MET-FAST-008-001	**21.8**
C	20	PU-SOL-THERM-009-001	**18.8**
E	88	LEU-SOL-THERM-007-003	**16.5**
A	99	U233-MET-FAST-002-002	**13.2**

- Calculations with MCNP-6.1
- Calculations with MCNP-6.1

Criticality Benchmarking – Mosteller's suite with 123 Benchmarks

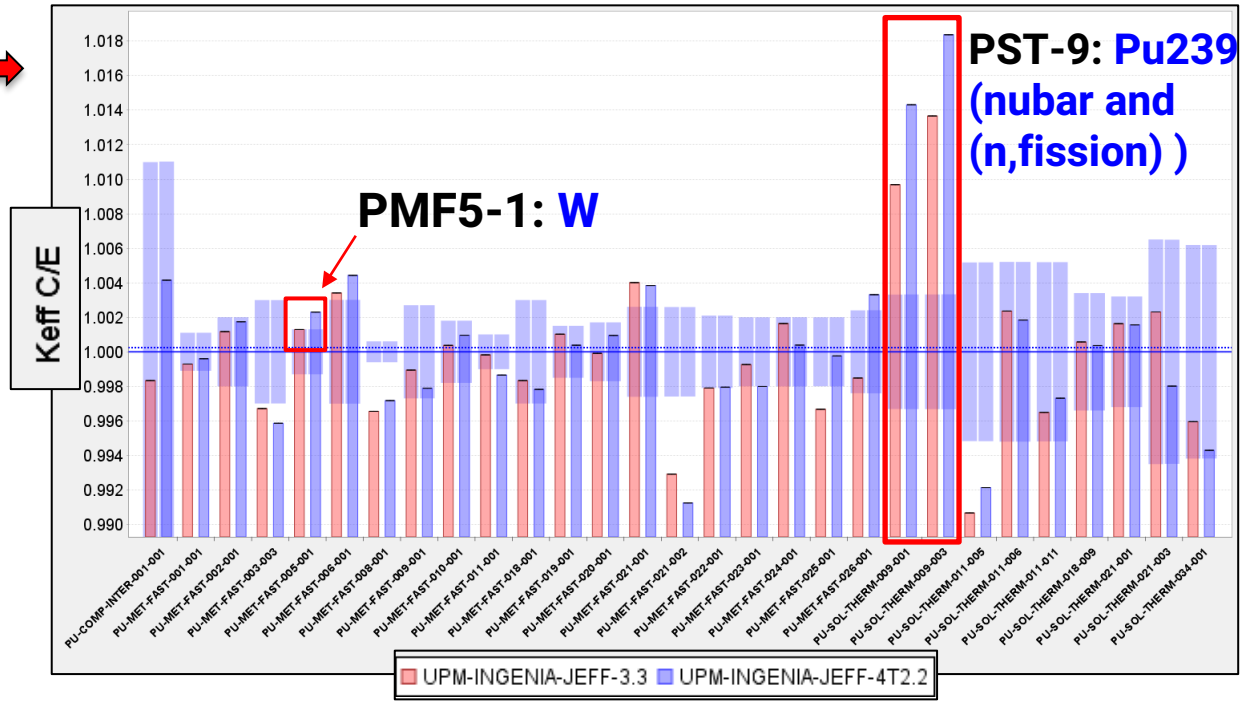
Criticality Benchmarking: Mosteller's Suite - 123

Table 3. Reduced-chi squared values in the Extended (123) Criticality Mosteller's suite

	JEFF-3.3	JEFF-4.0T0		JEFF-4.0T2
PU	3.05	3.13		**4.15**
HEU	2.64	**6.76**		**9.08**
IEU	3.33	4.29		2.75
LEU	2.14	2.60		**2.79**
U233	1.55	2.35		**2.37**
MIX	0.91	0.88		0.70
SPEC (C/E) Dexp=0.00340	0.99173	0.99479		0.99408
All	2.25	3.80		6.74

❑ Values predicted with **DICE tool -"keff trends plots"**

JEF/DOC-2041 *(O. Cabellos, "Overview of Processing, Verification and Benchmarking activities at UPM", 2021)*

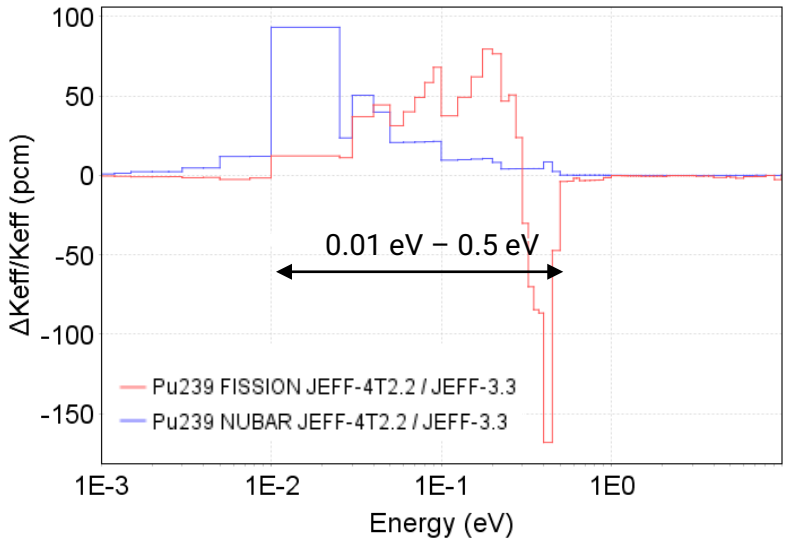


Criticality Benchmarking – Mosteller's suite with 123 Benchmarks

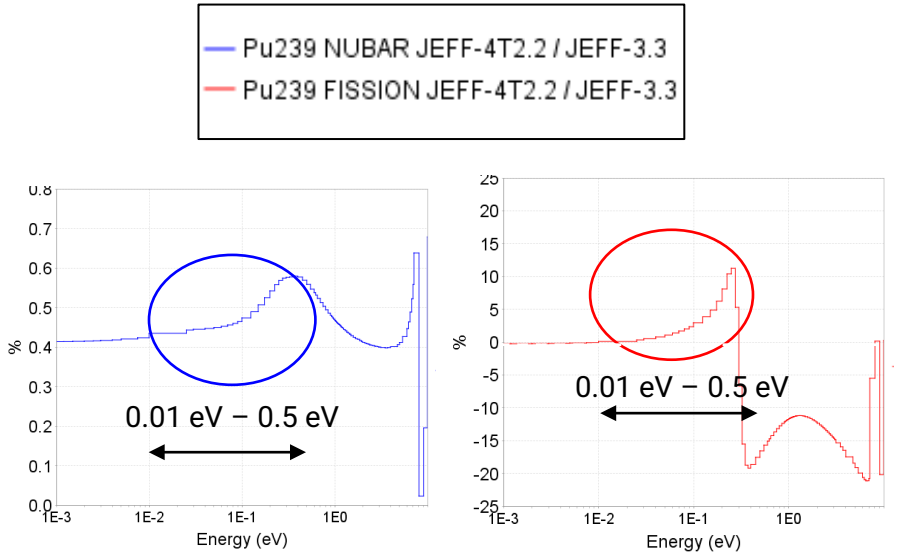
Sensitivity Analysis – NDaST perturbation Analysis … a very useful tool to find issues in the evaluation of ND!

			JEFF-4T2.2		JEFF-3.3		Δkeff (in pcm)		239Pu(nubar)	239Pu(n,fission)
CASE	keff-EXP	ExpUnc	Calc keff	Calc. Dkeff	Calc keff	Calc. Dkeff	J4T22 - J33		JEFF-4T2.2/JEFF-3.3	JEFF-4T2.2/JEFF-3.3
PU-SOL-THERM-009-003	1.0003	0.0033	1.01868	0.00005	1.01397	0.00005	+471		+455	+216
PU-SOL-THERM-009-001	1.0003	0.0033	1.01462	0.00006	1.00999	0.00006	+463		+455	+202

Δkeff/keff in PST-009-001 due to change in Pu239 (nubar) and (n,fission) JEFF-4T2.2 / JEFF-3.3

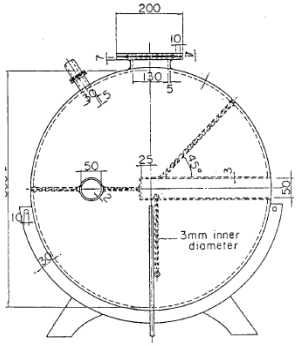


Pu239(nubar) and (n,fission) JEFF-4T2.2 / JEFF-3.3



Shielding Benchmarking

OKTAVIAN TOF Benchmarks (15 cases)

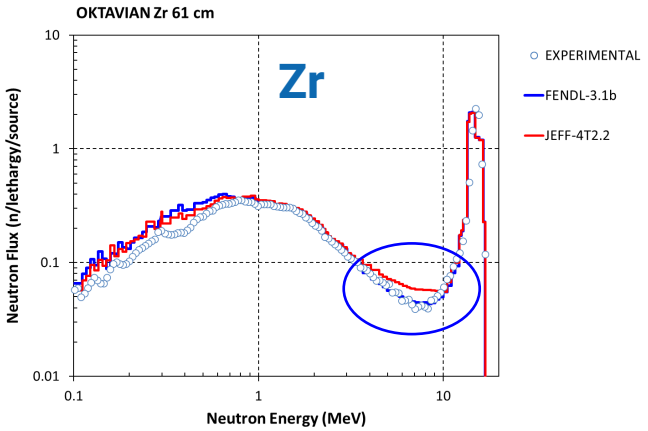


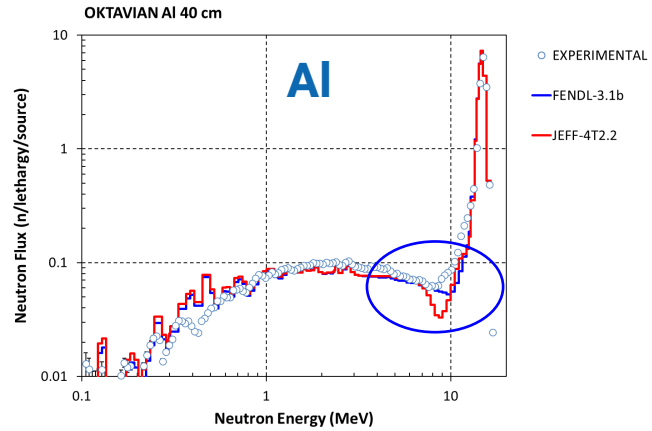
Neutron source spectra	
CASE 1 (Table 4.2)	LiF, Mn , Cu, Mo, W
CASE 2 (Table 4.3)	Teflon, Si, Co
CASE 3 (Table 4.4)	Al
CASE 4 (Table 4.5)	Ti, As, Se, Zr
CASE 5 (Table 4.6)	Cr, Nb

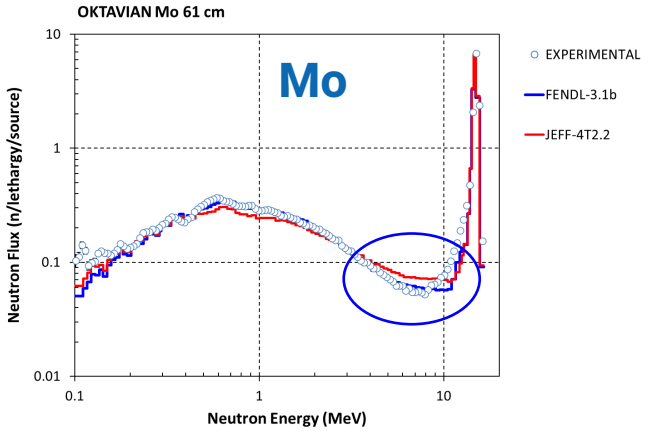
Figure: Neutron leakage from OKTAVIAN pulsed sphere Ex) 61 cm sphere: Type I

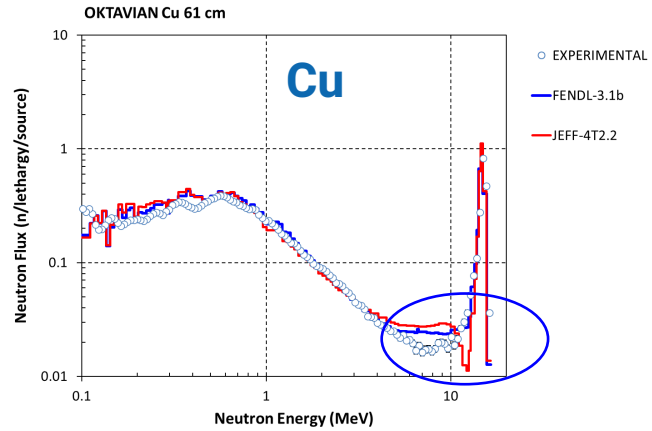
VESSEL GEOMETRY	Type-I 61 cm ø	Type-II 40 cm ø	Type-III 60 cm ø	Type-IV 28 cm ø
MATERIAL	Cu	Al	Si	Nb
	LiF	As		
	Mn	Co		
	Mo	Cr		
	Zr	Se		
		Teflon		
		Ti		
		W		

JEFF4T2 evaluations to be reviewed !









Reference: F. Maekawa et al., "Collection of Experimental Data for Fusion Neutronics Benchmark", JAERI, 1994.

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