TRIPOLI-4.4 - JEFF-3.1 & ENDF/B-VII b1 with the ICSBEP Criticality Models

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CADARACHE

Codes, libraries and benchmarks versions

- TRIPOLI-4.4.1, Monte Carlo, pointwise mode
- NJOY-99.90+ (111) and CALENDF-2005 (build 66)
- ENDF/B-VII b1 /GP (387) with **223 PT's in the URR** and /Th (20) files on the 24th October 2005
- JEFF-3.1/GP (381) **with 140 PT's in the URR** and /Th (9)
- International Handbook of Evaluated Criticality Benchmarks Experiment, ICSBEP **September 2005**
- On Bi-pro SUN Blade workstation

TRIPOLI-4.4

No spelling mistake,
Voltaire phraseology

Monte Carlo code

TRIPOLI : **TRI** dimensionnelle **POLI** cinétique

Five main classes of problems :
- Shielding studies
- Criticality studies
- Core physics studies
- Instrumentation
- Dosimetry

Particles:
- Neutrons
- Gamma
- electrons, positrons

Nuclear Data Libraries and Processing

NJOY-99.90+ on SUN workstation

1. Reconstruction at 0 K (RECONR)
2. Doppler Broadening at T K (BROADR)
3. Treatment of Unresolved Range (UNRESR)

Free Gas thermalisation is done within TRIPOLI-4.4.1

4. Treatment of Thermal Neutron scattering data for materials (THERMR)

Modification: results in terms of equi-probable cosines instead of equi-probable angles (on 32 bins)
MT's 221 and 222 hard coded

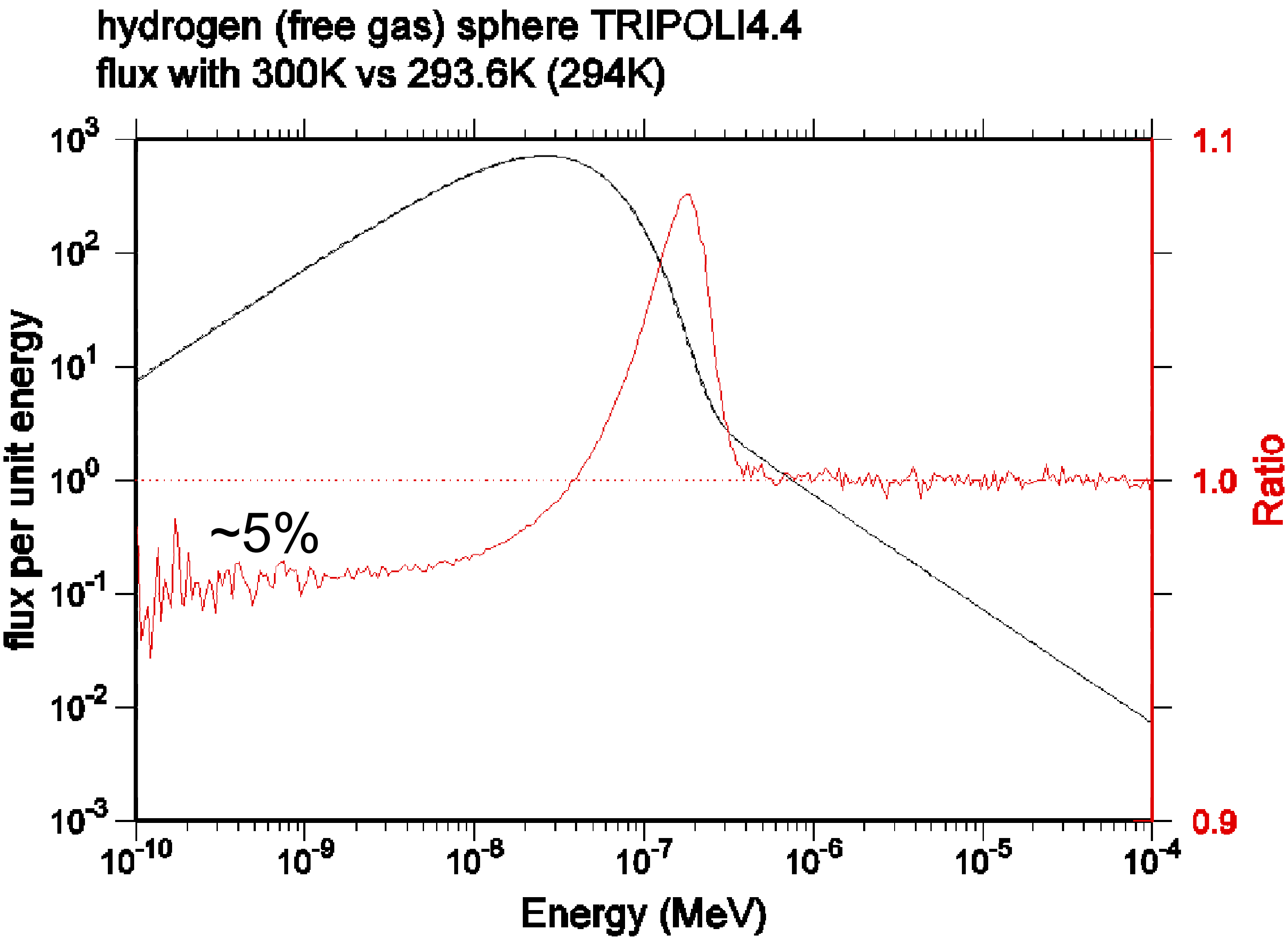
➔ Pointwise cross section

CALENDF-2005 on SUN workstation

1. Reconstruction, Doppler, URR

➔ Probability tables

Temperatures 294K versus 300K: neutron spectra



NJOY-99.90+ modules processing scheme

Evaluations

NJJOY-99.90

Modules	Main parameters	Outputs
moder		
reconr	err = 0.001 (0.1%)	
broadr	errthn = 0.001	Thermal quantities
unresr		
moder		pendf files
thermr	nbin = 32 tol = 0.001 emax = 4.95	
moder		

Tripoli-4.4.1 library

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Tripoli-4.4.1 Libraries

TRIPOLI-4.4.1 generates XDR portable binary and angular distribution files the first time it reads in a PENDF and and an ENDF file

Seven File Types are used :

1. Evaluation (ascii)
2. **PENDF (binary)**
3. Dictionary of cross sections (ascii)*
4. Binary XDR pointwise file*
5. Anisotropy file (ascii)*
6. **Probability tables (ascii)**
7. **Thermal file (ascii)**

*: generated by TRIPOLI the first time it access the data file.

140 in JEFF-3.1
223 in ENDF/B-VII b1

Tests for evaluations :

ENDF-102 format
Normalization (angular and energetic distribution)

T4XS-4.4.1 library files

jeff3.neutron.H1_H2O.bcd
jeff3.neutron.H1_H2O.bcd.therm
jeff3.neutron.H1_H2O.bcd.therm.294 (only at the file temperature)
jeff3.neutron.H1_H2O.bcd.aniso

jeff3.gamma.H1_H2O.bcd

Evaluation

jeff3.neutron.U238.bcd
jeff3.neutron.U238.bin.pendf.294
jeff3.neutron.U238.xdr.pendf.294.dictio
jeff3.neutron.U238.xdr.pendf.294
jeff3.neutron.U238.bcd.aniso
jeff3.neutron.U238.bcd.tp.294

Angular distribution

jeff3.gamma.U238.bcd

For each of the 390 isotopes in a single directory

TRIPOLI-4.4.1 libraries

file t4path.jeff3_1

/export/opt/CODE/TRIPOLI4.4.1/Env-4.4/jeff3_1.dictionary
/export/opt/CODE/TRIPOLI4.4.1/mass_rmd.mas95
/export/opt/CODE/TRIPOLI4.4.1/JEFF31/Qfission
/export/opt/CODE/TRIPOLI4.4.1/Mott_rutherford

Isotopic dictionary
Atomic mass
Fission Q values
Mott - Rutherford electron-positrons cross section

TRIPOLI-4.4.1 dictionary

File jeff3_1.dictionary

/export/opt/CODE/TRIPOLI4.4.1/JEFF31/T4XS-4.4
390

AC225	8925	8900	-1	jeff3.neutron.Ac225.bcd
AC226	8928	8900	-1	jeff3.neutron.Ac226.bcd
AC227	8931	8900	-1	jeff3.neutron.Ac227.bcd
AG107	4725	4700	-1	jeff3.neutron.Ag107.bcd

***

H1 125 100 -1 jeff3.neutron.H1.bcd
H1_H2O 125 100 1250001 jeff3.neutron.H1_H2O.bcd

***

U238	9237	9200	-1	jeff3.neutron.U238.bcd
V	2300	2300	-1	jeff3.neutron.V.bcd

**

ZR95	4040	4000	-1	jeff3.neutron.Zr95.bcd
ZR96	4043	4000	-1	jeff3.neutron.Zr96.bcd

TRIPOLI-4.4.1 input sequence

static_tripoli4-4.4 -d hmf001c2 -s TABPROB –c ~/Env-4.4/t4path.jeff3_1 -p graphe -t bsd >& hmf001c2.out

static_tripoli4-4.4 -d lct006c13 -s NJOY -c ~/Env-4.4/t4path.jeff3_1 -o lct006c13.res >& lct006c13.out

TRIPOLI use BSD socket under the GNU C library Lesser General Public License and so can access any CPU on a network without the need of message passing libraries

File graphe in the ./ directory

```
PROCESS
4
process  monitor  static_tripoli4-4.4   cade
process  scorer   static_tripoli4-4.4   cade
process  tache1   static_tripoli4-4.4   cade
process  tache2   static_tripoli4-4.4   cade
GRAPH
scorer <-> tache1
scorer <-> tache2
FIN
```

Sun dual-core
or
workstation

TRIPOLI-4.4.1 program and multi-processing

Networking Services Library Functions xdr(3NSL)

NAME

xdr - library routines for external data representation

DESCRIPTION

XDR routines allow C programmers to describe arbitrary data structures in a machine-independent fashion. Data for remote procedure calls (RPC) are transmitted using these routines.

Sockets Library Functions socket(3SOCKET)

NAME

socket - create an endpoint for communication

SYNOPSIS

```
cc [ flag ... ] file ... -lsocket -lnsl [ library ... ]
#include <sys/types.h>
#include <sys/socket.h>

int socket(int domain, int type, int protocol);
```

DESCRIPTION

socket() creates an endpoint for communication and returns a descriptor.

Angular distribution

- The angular distribution is computed by TRIPOLI-4.4.1 the first time a pendf file is accessed and the code require to be linked to the original endf file

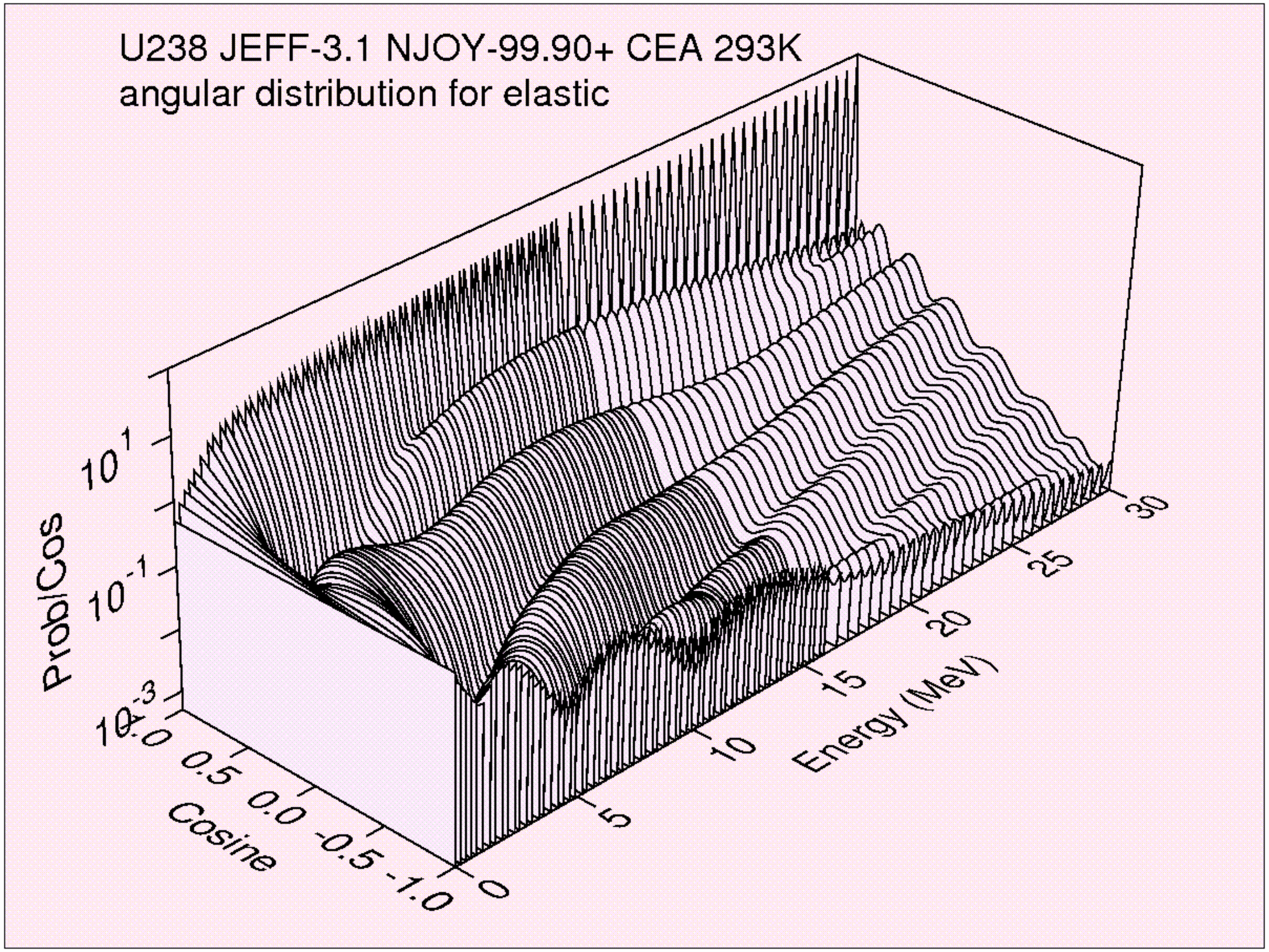
- The computed angular distribution is variable, file dependant and can contain up to 256 equally probable cosine bins

- For the JEFF-3.1 U238 the angular distribution have been produced by the ECIS optical model code and tabulated in 91 bins from 0 to 180 degree. It is used as such by TRIPOLI-4.4.1

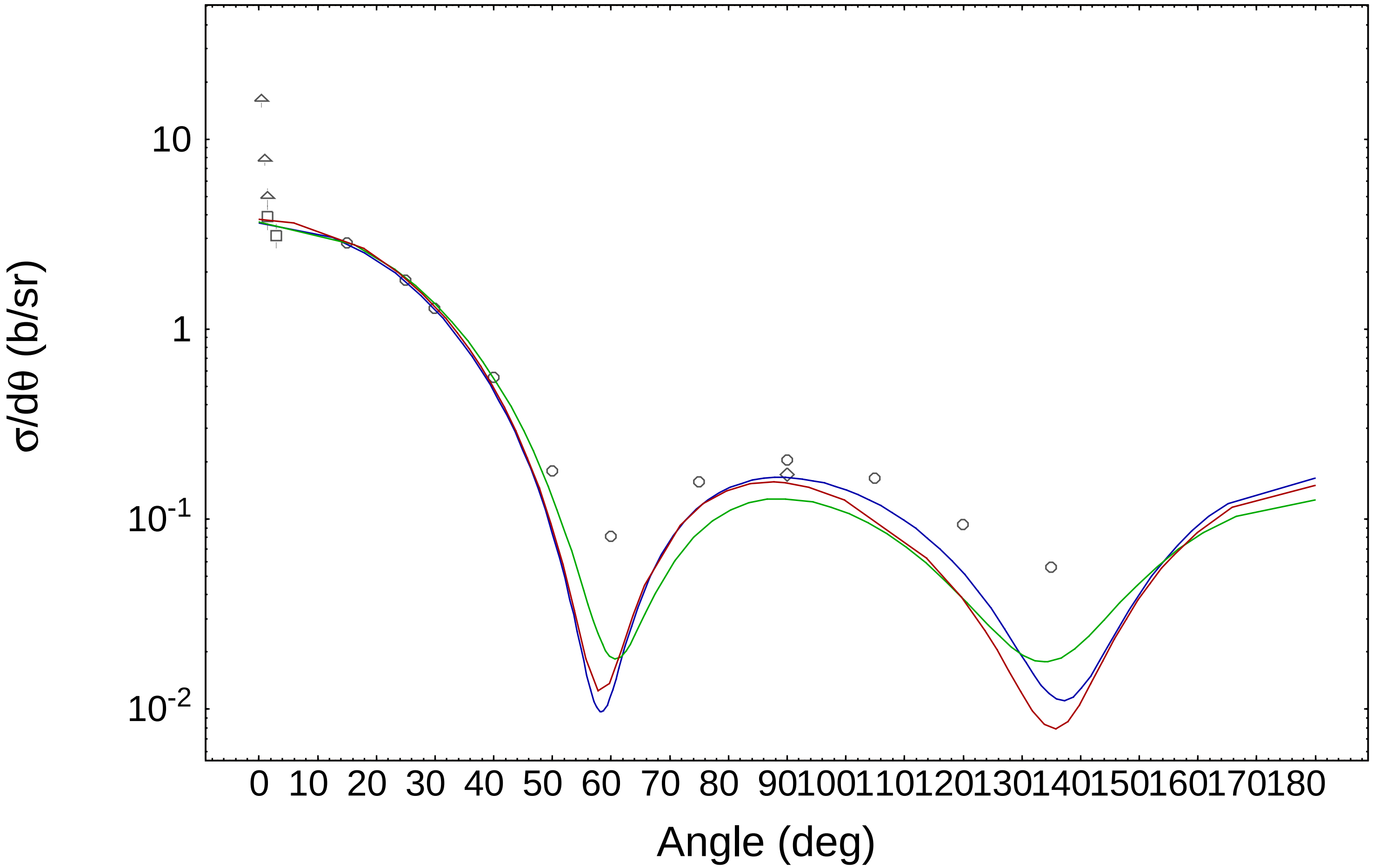
- Elastic and inelastic channels structures are preserved

- It is a much better representation than in Legendre coefficients

QA: MT=2 Angular distribution



U-238 elastic structure at 2.0 MeV



subtle differences between recent libraries

TRIPOLI-4.4.1 & JEFF-3.1 + Probability Table

- The probability table have been produced by CALENDF-2005 in 11276 groups, with IPRECI =4 (~0.002 accuracy)
- They can be used by TRIPOLI-4.4.1:
  - in the **U**nresolved **R**esonance **R**ange, **for 140 isotopes**
  - in the entire energy range, “PT sampling mode”
- The CALENDF probability table order vary from group to group

NOR vary from 1 to 11

NOR = table order; NPAR number of partials (four + (n.xn))
I = first negative moment

```
tables de probabilite pour  92-U -238 BRC,ORNL+  DIST-APR05
ZA=92238 MAT=9237 TEFF=294. 11276 groupes 1.0000E-5  1.9640E+7 IPRECI=4
IG 2148 ENG=2.237077E+5 2.241743E+5 NOR= 4 I= -3 NPAR=4 KP=2 101 18 4 0
1.094003-1  8.823080+0  8.196058+0  9.286816-2  1.266144-4  5.340267-1
4.538996-1  1.013560+1  9.196054+0  1.202600-1  1.263996-4  8.191575-1
4.029584-1  1.154104+1  1.023916+1  1.267343-1  1.261434-4  1.175020+0
3.374166-2  1.417834+1  1.326865+1  1.516819-1  1.255512-4  7.578883-1
Probability  Total       Elastic     Absorption  Fission     Inelastic
```

CALENDF-NJOY comparison for U238 at 293.6K

COMPARISON ON CROSS SECTION MT= 101 in the **U**nresolved **R**esonance **R**ange

LIST OF DIFFERENCES GREATER THAN 0.0100

	CALENDF	NJOY	EINF	ESUP	SIGMA GENDF	SIGMA P.T.	DELTA
16	833	1136	1.995887E+04	2.012589E+04	5.525137E-01	5.446610E-01	0.014418
17	832	1137	2.012589E+04	2.029431E+04	5.106446E-01	4.612736E-01	0.107032
18	831	1138	2.029431E+04	2.046413E+04	5.092291E-01	5.336834E-01	-0.045822
19	830	1139	2.046413E+04	2.063538E+04	5.078018E-01	5.269383E-01	-0.036316
20	829	1140	2.063538E+04	2.080806E+04	5.063609E-01	4.876923E-01	0.038279
21	828	1141	2.080806E+04	2.098218E+04	5.049111E-01	5.345675E-01	-0.055477
22	826	1143	2.115777E+04	2.133482E+04	5.019718E-01	4.831857E-01	0.038880
23	825	1144	2.133482E+04	2.151335E+04	5.004830E-01	5.126722E-01	-0.023776
24	824	1145	2.151335E+04	2.169338E+04	4.989832E-01	5.114362E-01	-0.024349
25	823	1146	2.169338E+04	2.187491E+04	4.974701E-01	5.028943E-01	-0.010786
26	822	1147	2.187491E+04	2.205796E+04	4.959444E-01	5.031609E-01	-0.014342
27	821	1148	2.205796E+04	2.224255E+04	4.944059E-01	4.763083E-01	0.037996
28	820	1149	2.224255E+04	2.242868E+04	4.928544E-01	5.078373E-01	-0.029503
29	819	1150	2.242868E+04	2.261636E+04	4.912901E-01	5.222933E-01	-0.059360
30	817	1152	2.280562E+04	2.299646E+04	4.881219E-01	4.805247E-01	0.015810
31	816	1153	2.299646E+04	2.318890E+04	4.865180E-01	4.499056E-01	0.081378
32	815	1154	2.318890E+04	2.338295E+04	4.849005E-01	5.166270E-01	-0.061411
33	814	1155	2.338295E+04	2.357862E+04	4.832695E-01	4.912039E-01	-0.016153
34	813	1156	2.357862E+04	2.377593E+04	4.816249E-01	4.320517E-01	0.114739
35	811	1158	2.397489E+04	2.417552E+04	4.782943E-01	4.857236E-01	-0.015295
36	810	1159	2.417552E+04	2.437782E+04	4.766081E-01	4.351625E-01	0.095242

****

ICSBEP leu-comp-therm-006 (JAERI)

Code				Tripoli-4.4		Tripoli-4.4	
Library				JEFF-3.1		ENDF/B-VII	S.D.
Release						b1	
ICSBEP						Thermal systems	
LCT-006		Exp.	Unc.				
	c-1	1.0000	200	1.00165	28	1.00014	24
	c-3	1.0000	200	1.00268	22	1.00134	19
	c-4	1.0000	200	1.00164	27	1.00007	24
	c-8	1.0000	200	1.00185	27	1.00078	24
	c-9	1.0000	200	1.00134	27	1.00030	24
	c-13	1.0000	200	1.00122	27	0.99967	24
	c-14	1.0000	200	1.00099	27	0.99958	24
	c-18	1.0000	200	1.00127	27	0.99973	24
Average				1.00158		1.00020	
Δ				158	-30	20	-125

In red and in the S.D. column the Δ with MCNP4c3 on the same benchmarks

Mean Δ Lib = 138 pcm with TRIPOLI-4.4
Mean Δ Lib = 95 pcm with MCNP4c3

 # ORNL4&5 # U-235 # H1

~150 pcm MCNP4c3 – TRIPOLI-4.4 bias remains, lib. independent due to # input decks, # thermal S(α,β) handling, this needs further investigation and explanation

ICSBEP leu-comp-therm-007 (VALDUC)

Case 1

22 x 22 rods; 484 rods

pitch = 1.26 cm

critical water height = 90.69 cm

Grid plate:

60 x 60 cm, 0.25 cm thick

Case 4

(Case 1 grid, with one rod each 2 holes)

18 x 17 rods; 306 rods

pitch = 1.26 x 2 = 2.52 cm

critical water height = 79.85 cm

Case 2

16 x 17 rods; 272 rods

pitch = 1.60 cm

critical water height = 73.53 cm

Grid plate:

60 x 60 cm, 0.25 cm thick

Case 3

15 x 15 rods; 225 rods

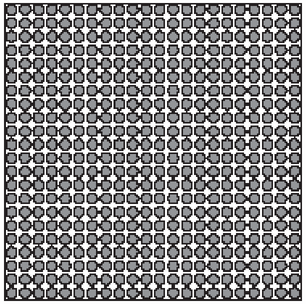
pitch = 2.10 cm

critical water height = 77.98 cm

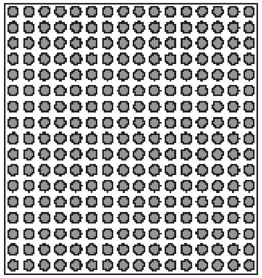
Grid plate:

60 x 60, 0.25 cm thick

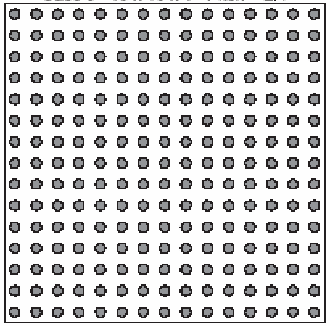
Case 1 22 x 22 x 1 Pitch = 1.26



Case 2 16 x 17 x 1 Pitch = 1.6



Case 3 15 x 15 x 1 Pitch = 2.1



Case 5

14 rods per side

547 rods

triangular pitch 1.35 cm

critical water height = 60.93 cm

Grid plate:

60 x 60 cm, 0.25 cm thick

Case 6

10 rods per side

271 rods

triangular pitch 1.72 cm

critical water height = 68.06 cm

Grid plate:

72 x 72 cm, 0.25 cm thick

Case 7

9 rods per side

217 rods

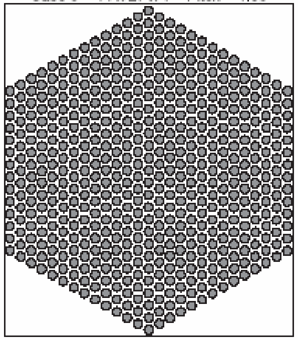
triangular pitch 2.26 cm

critical water height = 79.50 cm

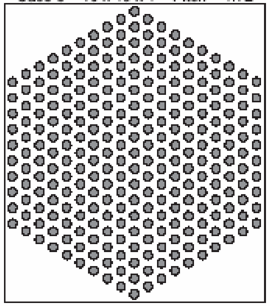
Grid plate:

92.5 x 92.5 cm, 0.25 cm thick

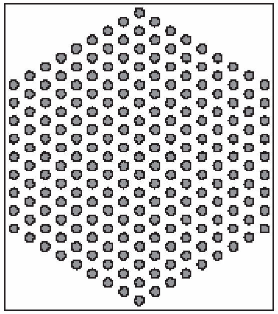
Case 5 14 x 27 x 1 Pitch = 1.35



Case 6 10 x 19 x 1 Pitch = 1.72



Case 7 9 x 17 x 1 Pitch = 1.9572

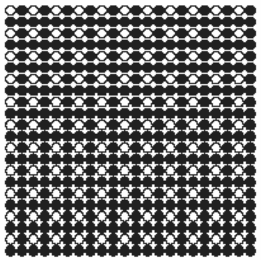


ICSBEP leu-comp-therm-007 & 039

Code				Tripoli-4.4		Tripoli-4.4	
Library				JEFF-3.1	S.D.	ENDF/B-VII	S.D.
Release						b1	
LCT-007							
Valduc	c-1	1.0000	160	0.99730	28	0.99616	24
	c-2	1.0000	160	0.99920	33	0.99807	30
	c-3	1.0000	160	0.99700	32	0.99635	30
	c-5	1.0000	160	0.99770	35	0.99588	30
	c-6	1.0000	160	0.99947	34	0.99817	30
	c-7	1.0000	160	0.99850	32	0.99690	30
Average				**0.99820**		**0.99692**	
Δ				**-180**		**-308**	
LCT-039							
Valduc	c-1	1.0000	140	0.99733	35	0.99590	30
	c-4	1.0000	140	0.99670	34	0.99512	29
	c-6	1.0000	140	0.99778	34	0.99661	30
Average				**0.99727**		**0.99588**	
Δ				**-273**		**-412**	

100 pcm low energy range library shift

 # U-235
 # H1


Case 6: 1 rod in 2 removed

ICSBEP leu-comp-therm-027 & 010

Code				**Tripoli-4.4**	
Library				**JEFF-3.1**	**S.D.**
Release					
LCT-027					
Pb	c-1	1.0000	110	1.00765	24
Δ				**765**	
LCT-10					
Pb	c-1	1.0000	210	1.00755	24
Δ				**755**	**608**
Pb	c-20	1.0000	280	1.00510	24
Δ				**510**	**420**

In red and in the S.D. column the Δ with MCNP4c3 on the same benchmarks

Lead reflected assemblies

ICSBEP heu-sol-therm

Code				Tripoli-4.4		Tripoli-4.4	
Library				JEFF-3.1	S.D.	ENDF/B-VII	S.D.
Release						b1	
Hiss		1.0000	600	1.00975	37	1.01084	37
Δ				975		1084	
Topsy-NI		1.0000	400	1.00280	49	1.00593	50
Δ				280		592	
Topsy-UR		1.0000	400	1.00688	46	1.00767	46
Δ				688		767	
HST001							
Mid	c-1	1.0000	250	0.99946	33	0.99896	33
Leakage	c-2	1.0000	250	0.99650	33	0.99534	34
Nitrate	c-3	1.0000	250	1.00295	33	1.00179	33
Sol.	c-4	1.0000	250	0.99890	33	0.99764	34
	c-5	1.0000	250	1.00001	33	0.99888	33
	c-6	1.0000	250	1.00347	33	1.00229	33
	c-7	1.0000	250	0.99892	33	0.99804	33
	c-8	1.0000	250	0.99920	33	0.99814	33
	c-9	1.0000	250	0.99496	33	0.99337	34
Average				0.99937		0.99827	
Δ				-63		-173	

JEF-2.2
+3000 pcm

U-235 B-VI r5
RRR impact

√

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ICSBEP heu-sol-therm

Code				Tripoli-4.4		Tripoli-4.4	
Library				JEFF-3.1	S.D.	ENDF/B-VII	S.D.
Release						b1	
HST010							
Fluo.	c-1	1.0000		1.00056	32	0.99949	32
Enrich.	c-2	1.0000		1.00132	33	0.99971	32
	c-3	1.0000		0.99828	32	0.99718	32
	c-4	1.0000		0.99671	33	0.99569	31
Average				**0.99922**		**0.99802**	
Δ				**-78**		**-198**	
HST011							
Fluo.	c-1	1.0000		1.00499	32	1.00357	32
Enrich.	c-2	1.0000		1.00130	32	1.00008	32
Average				**1.00314**		**1.00182**	
Δ				**314**		**182**	
HST012							
	c-1	0.9999	580	1.00163	32	1.00097	32
Δ				**173**		**107**	

√

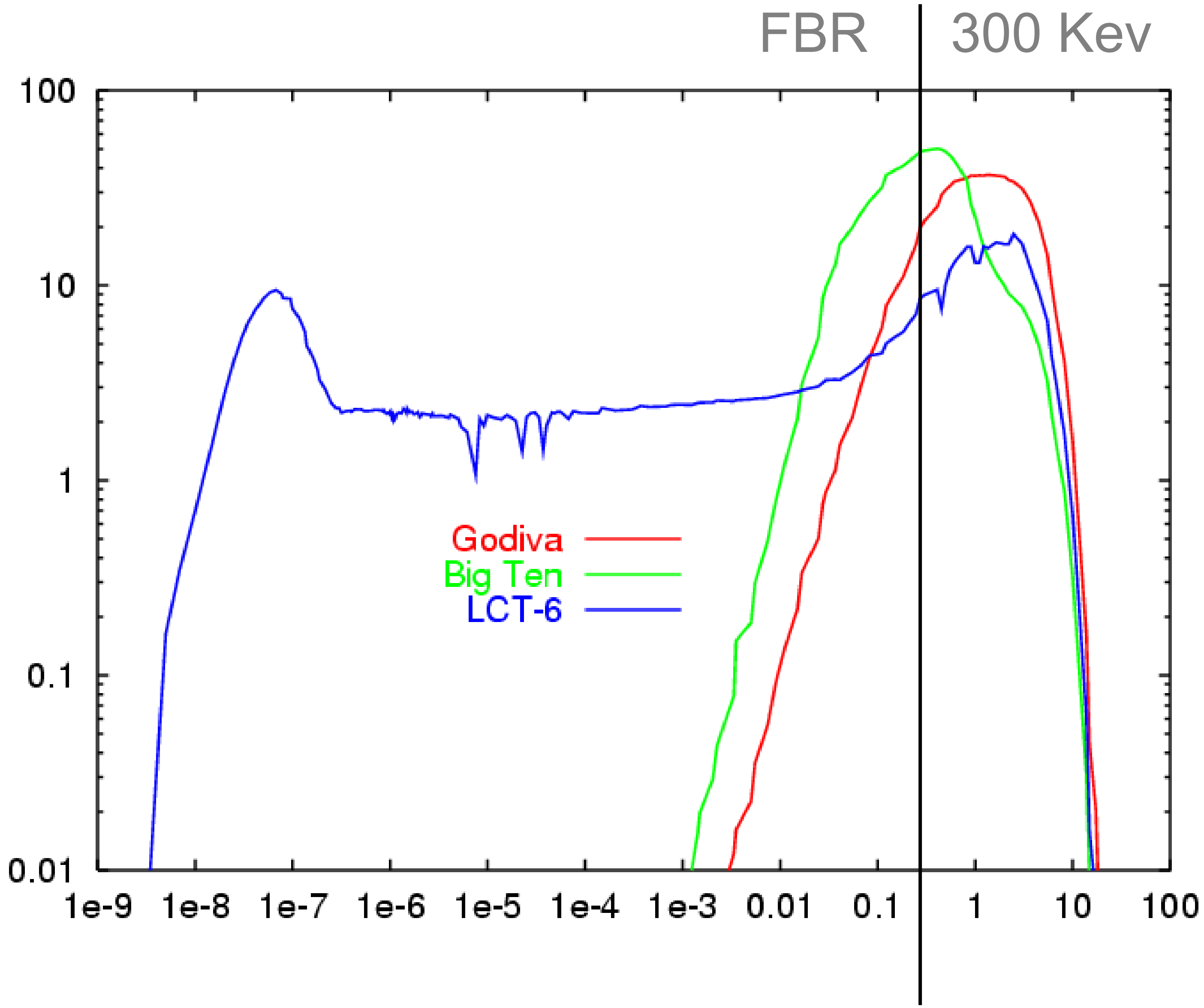
ICSBEP heu-sol-therm

Code				Tripoli-4.4		Tripoli-4.4	
Library				JEFF-3.1	S.D.	ENDF/B-VII	S.D.
Release						b1	
HST013							
ORNL-1	c-1	1.0012	260	0.99861	32	0.99819	32
ORNL-2	c-2	1.0007	360	0.99828	32	0.99768	32
ORNL-3	c-3	1.0007	360	0.99457	32	0.99371	32
ORNL-4	c-4	1.0003	360	0.99590	32	0.99522	32
Average				**0.99684**		**0.99620**	
Δ				**-346**		**-410**	
HST018							
Nitrate	c-1	1.0000	340	0.98886	33	0.98886	33
Sol. +	c-2	1.0000	460	0.98493	33	0.98416	33
Gado	c-3	1.0000	460	0.98857	33	0.98774	32
Average				**0.98745**		**0.98692**	
Δ				**-1255**		**-1308**	
HST019							
	c-1	1.0000	570	0.99671	32	0.99609	34
Δ				**-329**		**-391**	
HST032							
ORNL-10		1.0015	260	0.99950	32	0.99792	32
Δ				**-200**		**-358**	

√

Consistent under-prediction

Thermal and Intermediate energy benchmarks spectra



ICSBEP -met-fast-

Code				Tripoli-4.4		Tripoli-4.4	
Library				JEFF-3.1	S.D.	ENDF/B-VII	S.D.
Release						b1	
ICSBEP						Fast systems	
IMF-007							
Big Ten	deta.	1.0045	70	0.99863	25	1.00550	26
	simp.	1.0045	70	0.99781	25	1.00458	26
Δ				-628	583	54	86
	t.z.h.	0.9948	130	0.98853	24	0.99607	25
Δ				-627	670	127	45
IMF-012							
ZPR(16%)	c-1	1.0007	270	1.00225	25	1.00397	26
Δ				155	186	327	314
IMF-10							
ZPR-U9	c-1	0.9954	240	0.99223	24	0.99780	25
Δ				-317	-487	240	71
IMF-002							
	c-1	1.0000	300	0.99241	21	0.99988	21
Δ				-759	-787	-12	-51
IMF-001							
Jemima	c-2	1.0000	120	0.99784	25	1.00119	
	c-3	1.0000	100	0.99700	24	1.00120	
	c-4	1.0000	100	0.99841	24	1.00205	
Average				0.99775		1.00148	
Δ				-225	-167	148	78

ZPRs exp. results reliability ?

In red and in the S.D. column the Δ with MCNP4c3 on the same benchmarks

~600 pcm shift in the right direction in the fast range for B-VII b1

U-235 & U-238 in the continuum cross-section and angular distribution

No bias between TRIPOLI-4.4.1 & MCNP4c3

CADARACHE

ICSBEP -met-fast-

Code				Tripoli-4.4		Tripoli-4.4	
Library				JEFF-3.1	S.D.	ENDF/B-VII	S.D.
Release						b1	
HMF-028							
Flattop-25		1.0000	**300**	1.00157	23	1.00326	23
Δ				**157**	**159**	**326**	**295**
HMF-001							
Godiva	c1	1.0000	100	0.99650	23	1.00031	23
	c2	1.0000	100	0.99677	23	1.00003	23
Average				**0.99664**		**1.00017**	
Δ				**-336**	**-345**	**17**	**-40**
PMF-001							
Jezebel	c-1	1.0000	200	1.00003	30	1.00018	30
Δ				**3**	**-8**	**18**	**1**
PMF-002							
Jez. 240	c-1	1.0000	200	1.00418	30	0.99994	30
Δ				**418**	**430**	**-6**	**59**

In red and in the S.D. column the Δ with MCNP4c3 on the same benchmarks

Pu-239 fast √

U-235 B-VI r5
+ 300 pcm high energy
with ENDF/B-VII b1 or BRC

Pu240, differences in URR and continuum of JEFF-3.1

Conclusions (Monte Carlo)

TRIPOLI-4.4 - MCNP4c3 & JEFF-3.1 - ENDF/BVII b1

The keff's prediction do not **always** agree, particularly in the thermal range but the differences are within the experimental uncertainties. Nevertheless, those differences require further investigation and explanation

An excellent agreement exists in the fast range, whatever the libraries, when using Monte Carlo codes with CALENDF or PURR probability tables

One cannot help noticing numerous and large compensation effects, arising not only from the major isotopes such as U, PU but also from the minor ones including the structural isotopes

Times as come for the Monte Carlo benchmarking to probe further the basic data: angular distribution, emitted spectra, neutron spectrum and cross section ratio

Conclusions (JEFF-3.1/GP and /Th)

Not only capture or absorption, fission and nubar are important but elastic and inelastic levels AND their angular distribution needs to be known with a higher accuracy and exploited appropriately

The never quite finished standards need to find there ways into JEFF-3.x:

- U-235 (n,f) th + 150 KeV - 200 MeV,
- U-238 (n,f) 1.0 Mev - 200 MeV, (n,g) th +150 KeV - 2.2 MeV (recom.)
- Pu-239 (n,f) th +150 KeV – 200 MeV
- Au-197(n,g) th +250 KeV – 2.8 MeV
- Li6 (n,t)=(n,a) th +150 KeV – 2.8 MeV
- B-10 (n,a0,a1) th +150 KeV – 1.0 MeV

The benchmarking focus usually on only one energy range: thermal, intermediary or fast and the conclusion that can be drawn from it only apply to one range at a time