DE LA RECHERCHE À L'INDUSTRIE

Reactivity effect breakdown calculations with perturbations analysis – JEFF-3.1.1 to JEFF-3.2T1 application

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www.cea.fr

Outline

Context and goals

Selected benchmarks

Analysis methods

Results for JEFF-3.1.1 to JEFF-3.2T1 library change and perturbation analysis

Conclusion and outlook

Context and goals

Selected benchmarks

Context and goals

JEFF-3.2T1 library

- JEFF-3.2T1 library includes BRC-2009 actinides evaluation files
  - ^{234}U ^{235}U ^{236}U ^{238}U ^{239}Pu ^{240}Pu ^{241}Am .

- Collaborative work between units in CEA to produce unique evaluation files for nuclear community
  - First step : to define a common selected set of benchmarks
    Calculation with JEFF-3.1.1 and BRC-2009 evaluations (This work)
  - Second step : to build new common evaluation files from the existing ones
    Proposition to JEFF project for new JEFF-3.2 library
  - Third step : to share model parameters and models
    Production of new common evaluations

```
[ BRC2009    transport file : neutron  + 235U  1.e-5 eV -  30 MeV    99 0  0    0
 9.223500+4 2.330248+2          1          1          0          19228 1451    1
 0.000000+0 0.000000+0          0          0          0          69228 1451    2
 1.000000+0 3.000000+7          1          0         10          09228 1451    3
 0.000000+0 0.000000+0          0          0        195        1479228 1451    4
 92-U -235 BRC        EVAL-JUL08 P. Romain, B. Morillon, H. Duarte9228 1451    5
 BRC2009              DIST-      REV1-                            9228 1451    6
----BRC2009           Material 9228         REVISION 1            9228 1451    7
-----Incident neutron  data                                       9228 1451    8
------ENDF-6 Format                                               9228 1451    9
*********************************************************************9228 1451   20
                                                                   9228 1451   28
MF=1 General Information                                           9228 1451   29
                                                                   9228 1451   30
   The prompt fission neutron multiplicity and spectra             9228 1451   31
```

Context and goals

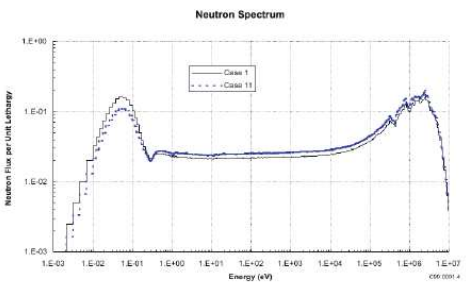
- Most important actinides
  ^{235}U ^{238}U ^{239}Pu ^{240}Pu .

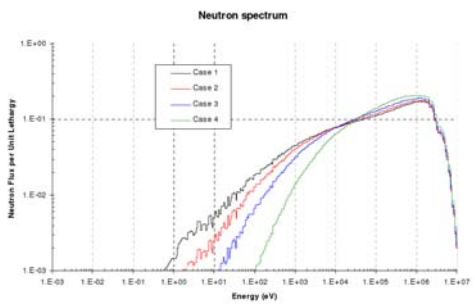
- Classical constraints concerning validation :
  - Criticality cases
  - Current reactors (PWR France)
  - Future reactors (SFR)

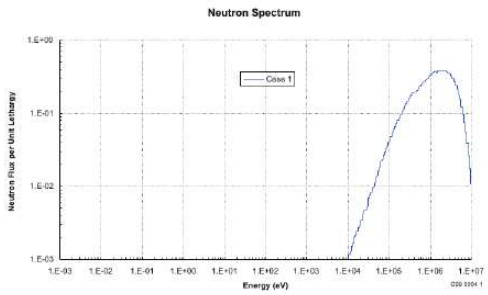
Selected benchmarks

	Type	Benchmark
U	ICSBEP	HMF Godivas, … IMF HxI Zeus, … HST
	ExperimentalReactors	EOLE Creole MASURCA 1B
Pu	ICSBEP	PMF Jezebels, PST
	Experimental Reactors	SNEAK 7A- 7B ZPPR 10A

- Many neutron spectra : THERMAL, INTERMEDIATE, FAST







Analysis methods

Deterministic methods (ECCO/ERANOS and PARIS)

- Based on the exact perturbation theory – exact formulation

$$(A - \frac{F}{k_{eff}})\Phi = 0$$

$$F\phi(\mathbf{r},\mathbf{\Omega},E) = \frac{\chi(E)}{4\pi} \times \int\int \nu_f(\mathbf{r},E',\mathbf{\Omega}'\Phi(\mathbf{r},\mathbf{\Omega}',E') \times d\mathbf{\Omega}' \times dE'$$

$$A\Phi(\mathbf{r},\mathbf{\Omega},E) = \mathbf{\Omega}\cdot\nabla\Phi(\mathbf{r},\mathbf{\Omega},E) + \Sigma_t\Phi(\mathbf{r},\mathbf{\Omega},E) - \int\int \Sigma_s(\mathbf{r},E' \to E,\mathbf{\Omega}' \to \mathbf{\Omega})\Phi(\mathbf{r},\mathbf{\Omega}',E') \times d\mathbf{\Omega}' \times dE'$$

where $\phi(\mathbf{r},\mathbf{\Omega},E)$ and $\phi^+(\mathbf{r},\mathbf{\Omega},E)$ are the direct and adjoint angular fluxes

- Reactivity variation can be expressed

$$d\rho = \frac{dk_{eff}}{k_{eff}^2} = -\frac{< \Phi^+, (dA - \frac{dF}{k_eff})\Phi >}{< \Phi^+, F\Phi >}$$

- and

$$\delta\rho_{(1)\to(2)} = -\frac{< \Phi^+_{(1)}, (\delta A - \frac{\delta F}{k_{eff2}})\Phi_{(2)} >)}{< \Phi^+_{(1)}, F_1\Phi_{(2)} >}$$

Analysis methods

Deterministic methods (ECCO/ERANOS and PARIS)

$$\delta\rho_{(1)\rightarrow(2)} = -\frac{< \Phi^{+}_{(1)}, (\delta A - \frac{\delta F}{k_{eff2}})\Phi_{(2)} >)}{< \Phi^{+}_{(1)}, F_1 \Phi_{(2)} >}$$

- Reference (1) adjoint flux is calculated with JEFF-3.1.1

  And perturbed (2) direct flux is calculated with BRC-2009

- ECCOLIBs processing is ensured to be the same

  NJOY CALENDF MERGE GECCO

  BRC-2009 produced on the basis of JEFF-3.1.1

  P5 anisotropy library (main actinides, moderators, structures materials)

  → homogeneous geometries only

- δA and δF calculations are performed by ERANOS or PARIS

- $\delta\rho_{(1)\rightarrow(2)}$ is given per reaction type, energy group, angular moment (for diffusion sections)

Stochastic methods (TRIPOLI-4)

- Complete isotope evaluation file and cross sections files replacement

  A simple way to analyze the effect of one isotope

- Partial data in evaluation file replacement

  For independent data (ν, χ, pdfs $f(\mu)$, …)

  Direct change in evaluation file (TRIPOLI-4 reads the original file)

- Correlated samples perturbation method

  Microscopic cross section perturbation (or density) in TRIPOLI-4

  $\sigma_{pert} = \lambda \times \sigma_{ref}$ with λ constant in group $[E_g, E_g+1]$

  λ calculated with a specific tool from two PENDF files

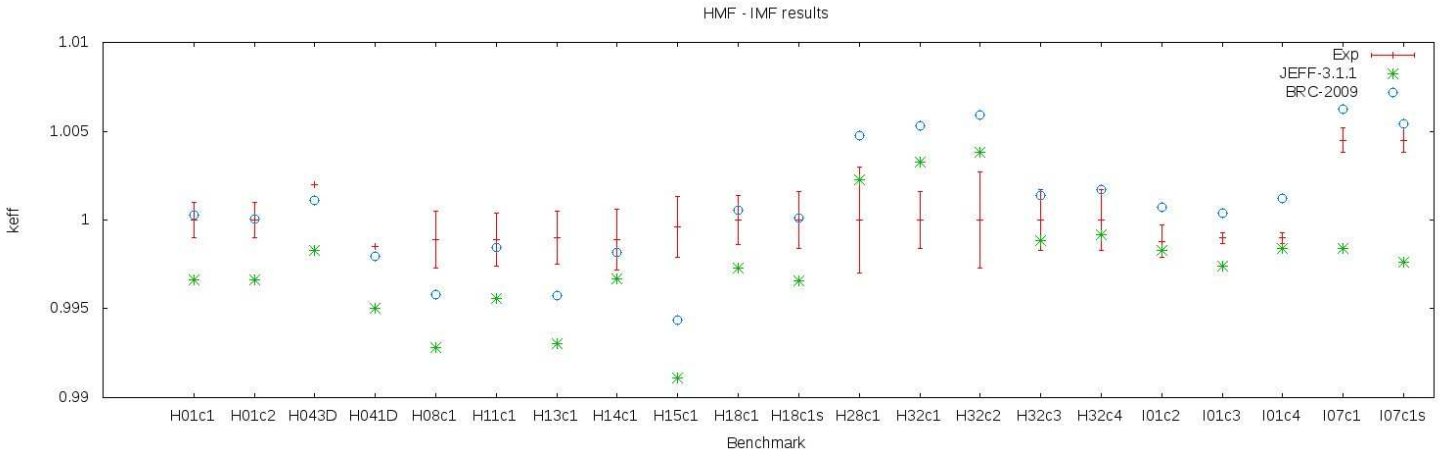
Results : fast spectrum

- HMF and IMF
- H(C,M,S)I
- PMF

ICSBEP experiments

- Experimental reactors

HMF and IMF results



- HMF and IMF results

  About +280 pcm as mean effect for HMF : a global better behaviour compared to experiment

Isotope	(n, γ)	ν	χ	(n, f)	(n, n)	(n, n')	(n, Xn)	Total
^{235}U								
PARIS	127	-838	2	323	8	558	192	**+371**
TRIPOLI-4	130 (1)	-835 (13)	x	310 (2)	26 (9)	x	156 (2)	**+365 (14)**
Discrepancy	+3 (1)	+3 (13)	x	-13 (2)	+18 (9)	x	36 (2)	**-6 (14)**
^{238}U								
PARIS	4	-28	1	22	-15	7	7	**-2**
TRIPOLI-4	4 (0)	-16 (13)	x	24 (1)	-17 (2)	x	0 (0)	**+14 (14)**
Discrepancy	0 (0)	+12 (13)	x	+2 (1)	-2 (2)	x	-7 (0)	**+16 (14)**
Total								
PARIS	131	-866	3	345	-7	565	199	**+369**
TRIPOLI-4	x	x	x	x	x	x	x	**+379 (20)**
Discrepancy	x	x	x	x	x	x	x	**+10 (20)**

(n, n') cannot be calculated with TRIPOLI-4 for all levels, and so for total inelastic
→ different inelastic thresholds
20th level

BRC-2009 370,6 keV
JEFF-3.1.1 393,2 keV

(n, n) calculated in two times
→ anisotropy with direct calculations
→ cross section with perturbation calculation

HMF001 - ECCO/ERANOS anisotropy : P5

HMF and IMF results

- HMF001 results

Nuclear data impact

Isotope	(n, γ)	ν	χ	(n, f)	(n, n)	(n, n')	(n, Xn)	Total
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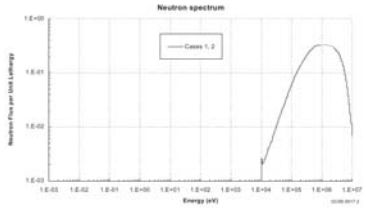
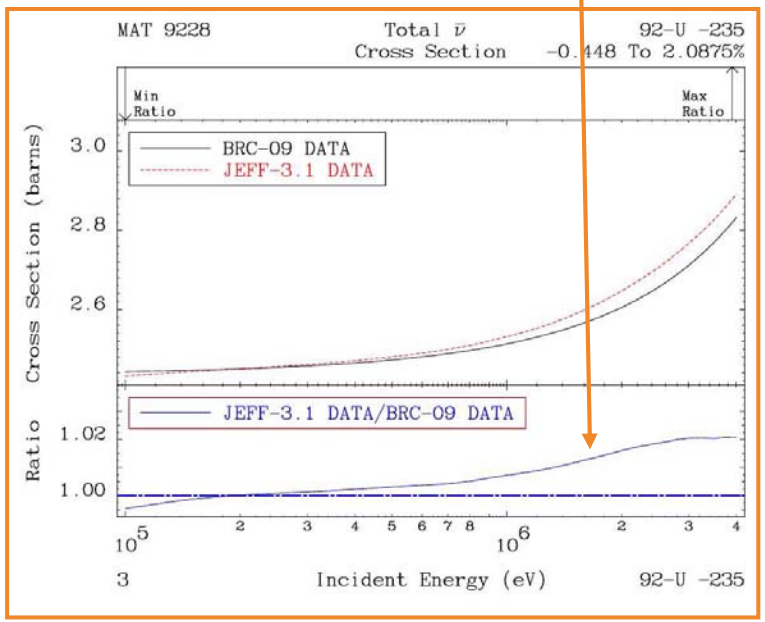
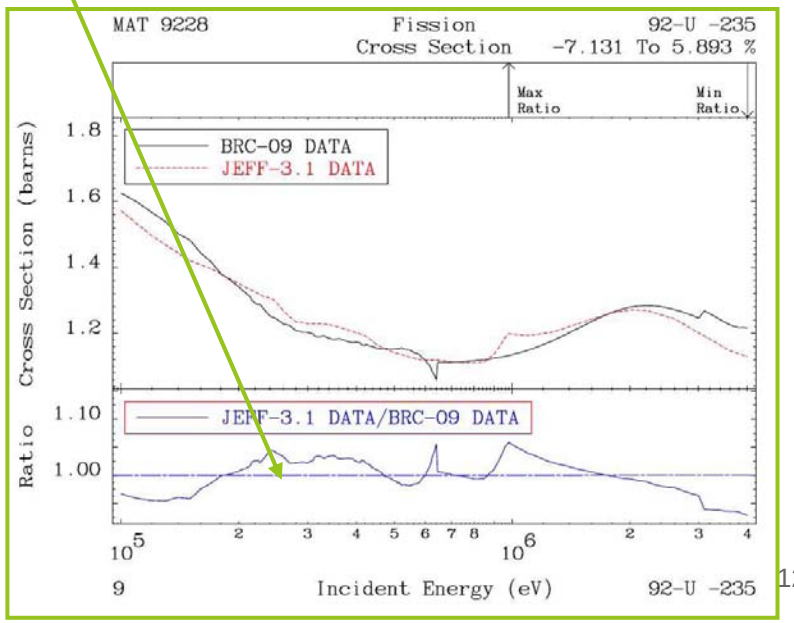


Spectrum
94,4% fissions
above 100 keV

Ratio Jeff/ Brcc

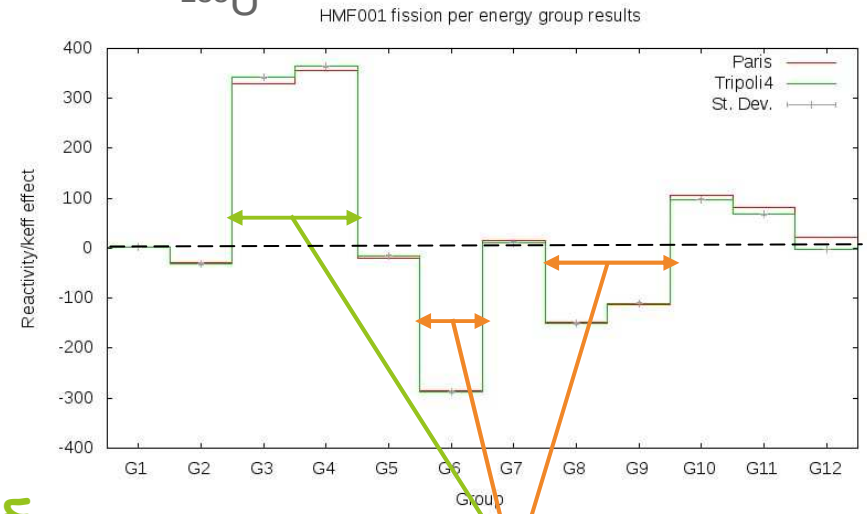




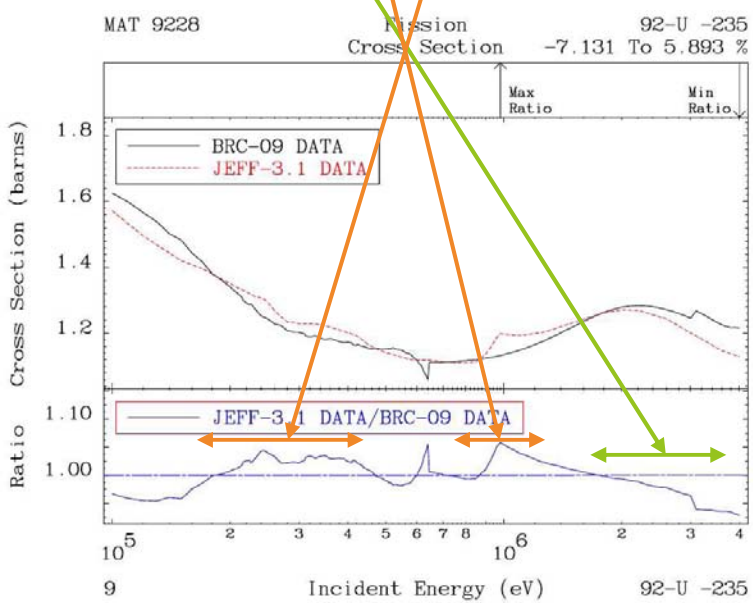
HMF 001 analysis

- HMF 001 results per reaction type and energy group : CEA RNR 33 groups mesh

^{235}U



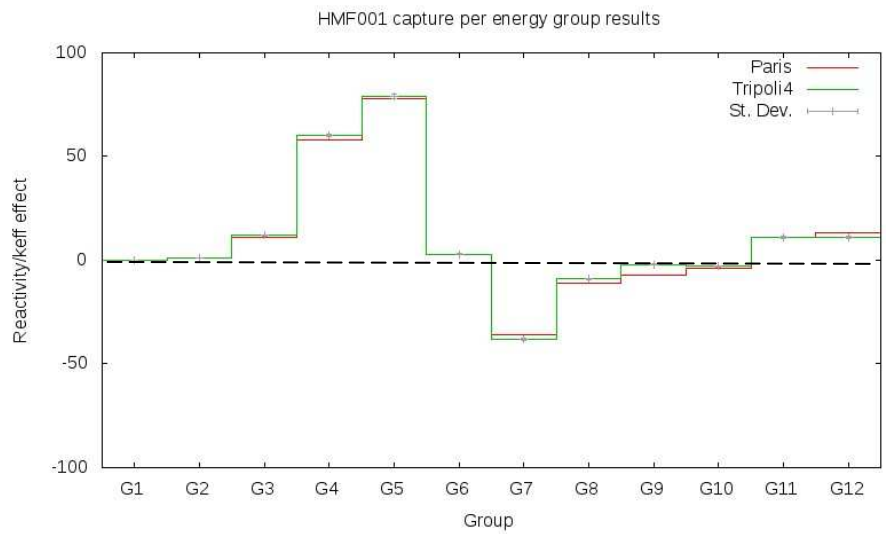
Fission



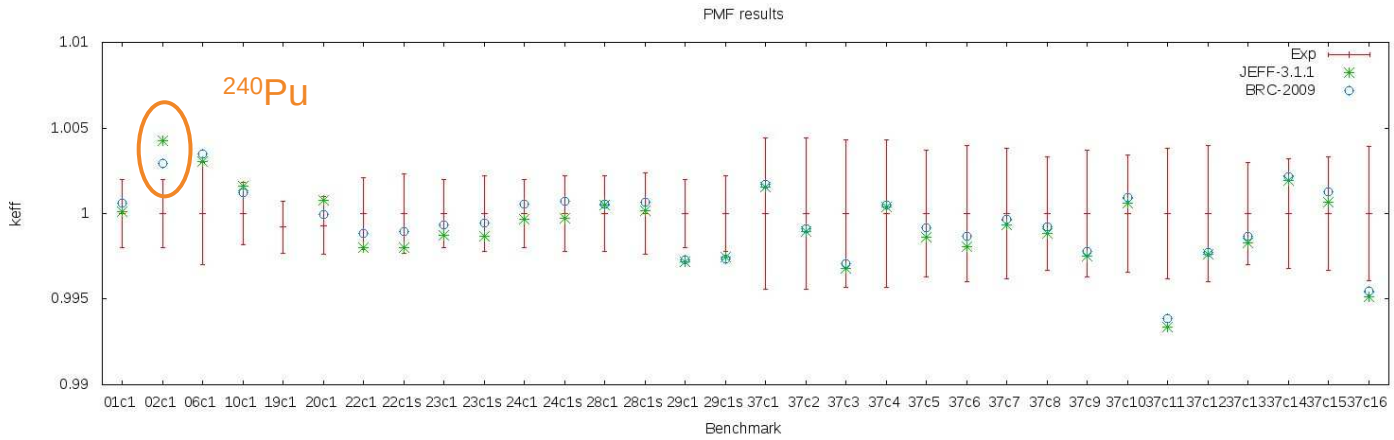
Ratio Jeff/ Brcc

Energy groups (MeV)
19,640 – 10,000 - 6,065
3,679 - 2,231 - 1,353
0,821 - 0,498 - 0,302
0,183 – 0,111 -0,067
0,041

Capture



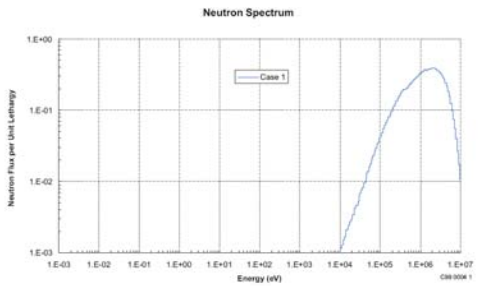
PMF results



- PMF results

  About +30 pcm as mean effect for PMF : a maximum effect for ^{240}Pu JEZEBEL close to -130 pcm

Isotope	(n, γ)	ν	χ	(n, f)	(n, n)	(n, n')	(n, Xn)	Total
^{239}Pu								
PARIS	-80	89	5	20	-93	160	28	**+129**
TRIPOLI-4	-78 (0)	+75 (11)	x	4 (1)	-92 (8)	x	10 (1)	**+112 (11)**
Discrepancy	+2 (0)	-14 (11)	x	-16 (1)	+1 (8)	x	-18 (1)	**-17 (11)**
^{240}Pu								
PARIS	-14	-70	-2	32	-7	8	1	**-2**
TRIPOLI-4	-14 (0)	-78 (11)	x	35 (1)	-7 (1)	x	0 (0)	**-41 (11)**
Discrepancy	0 (0)	-8 (11)	x	+3 (1)	0 (1)	x	-1 (0)	**-39 (11)**
Total								
PARIS	-94	19	3	52	-100	168	29	**+77**
TRIPOLI-4	x	x	x	x	x	x	x	**+53 (11)**
Discrepancy	x	x	x	x	x	x	x	**-24 (11)**



97,7% fissions above 100 keV

PMF001 - ECCO/ERANOS anisotropy : P5

PMF 001 analysis

- PMF001 results

Isotope	(n, γ)	ν	χ	(n, f)	(n, n)	(n, n')	(n, Xn)	Total
^{239}Pu								
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Discrepancy	0 (0)	-8 (11)	x	+3 (1)	0 (1)	x	-1 (0)	**-39 (11)**
Total								
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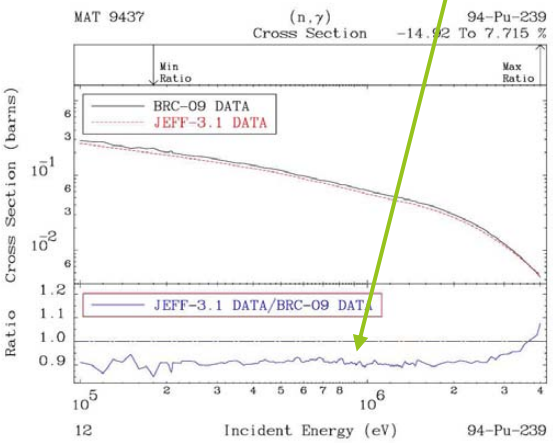
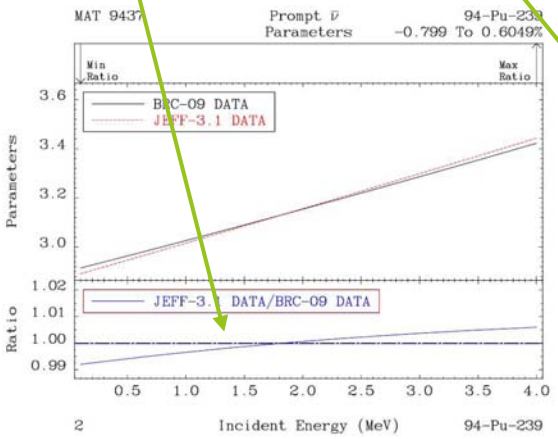
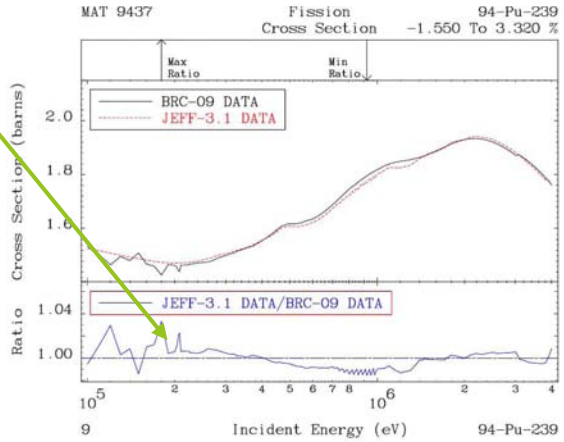
Discrepancy	x	x	x	x	x	x	x	**-24 (11)**





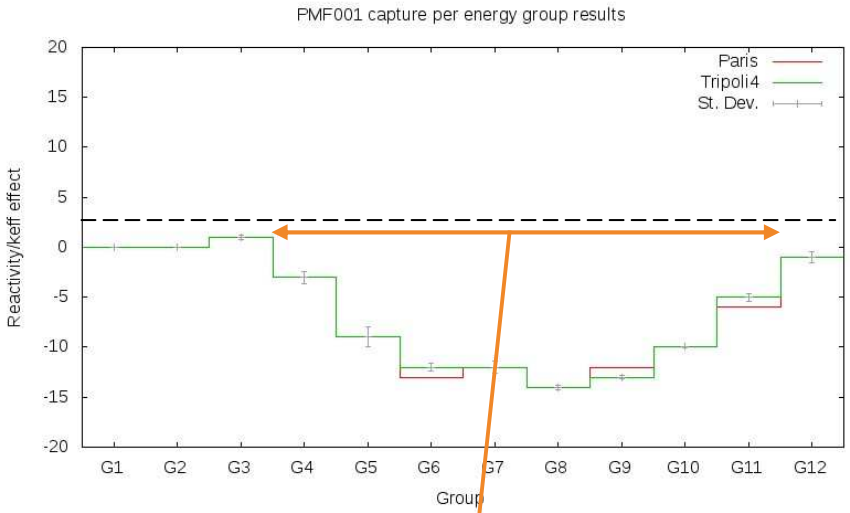


PMF001 analysis

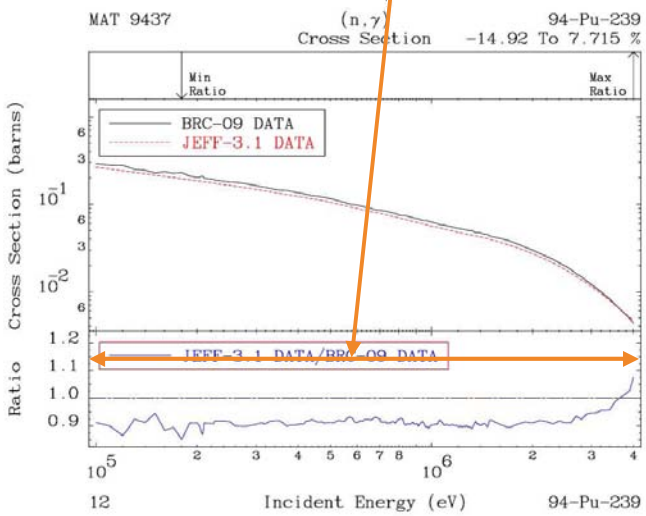
- PMF001 results per reaction type and energy group : CEA RNR 33 groups mesh

^{239}Pu

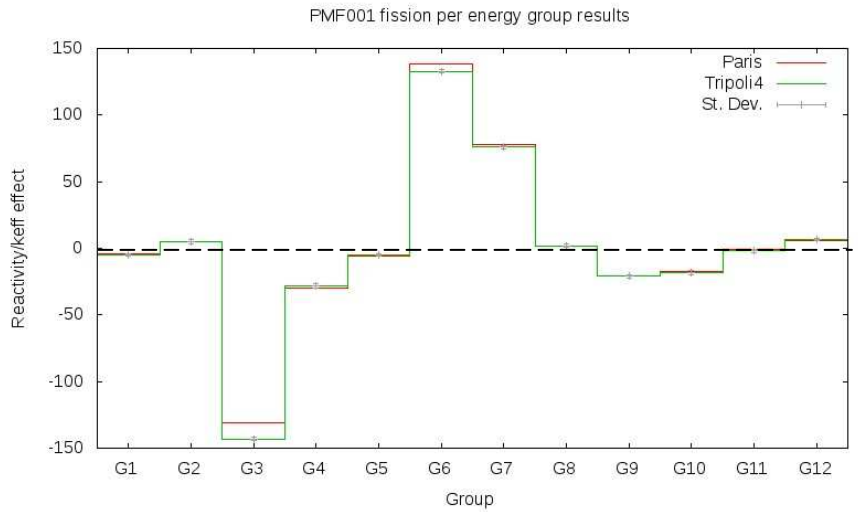
Capture



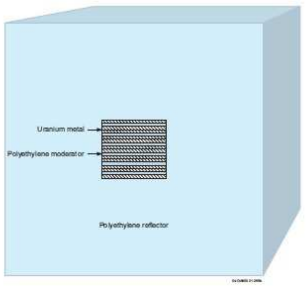
Ratio Jeff/ Brcc

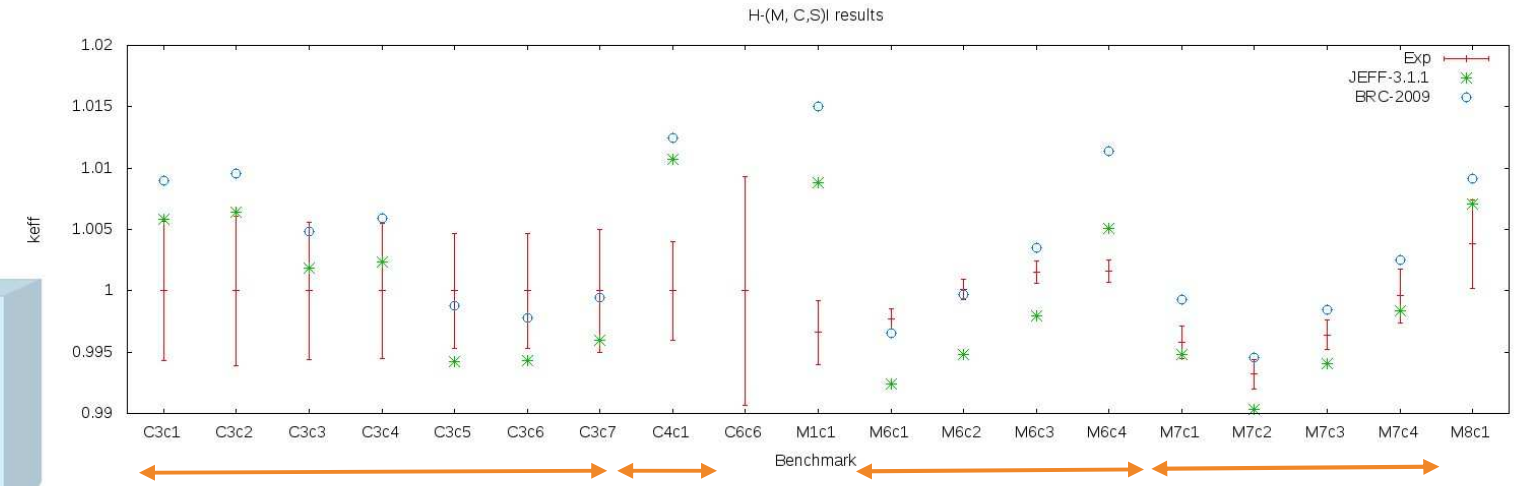


Fission



H(M-C-S)I results





UH3 cyl. COMET Exp.

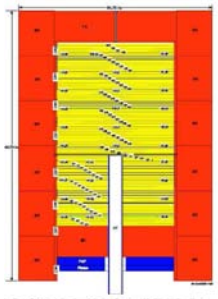
HECTOR Exp.

ZEUS Exp.

U moderated Slabs Exp.

- H(M-C-S)I results
  - HCI003 : ~ 2 to 4 keV
  - HCI004 : ~ 100 eV
  - HCI006 : ~ 6 keV
  - HMI006 : ~ 4, 9, 23 81 keV
  - HMI007 : ~ 2, 3, 4, 6 keV

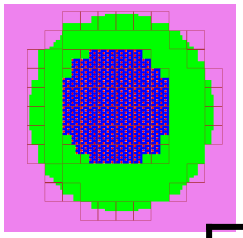
About +300 pcm as mean effect for H*I



Modelisation may be difficult with ECCO : calculation schemes needed Stochastic solution

Additional benchmarks for intermediate energies testing : (more representative of SFR spectra)

MASURCA 1B results



MASURCA-1B analysis

TRIPOLI-4.6

JEFF-3.1.1

PARIS/SNATCH P1

Isotope	(n, γ)	ν	χ	(n, f)	(n, n)	(n, n')	(n, Xn)	Total
^{235}U	+285	-44	+0	+241	-1	+72	+24	+577
^{238}U	-91	-356	+0	+227	+78	+50	+1	-91
Total	+193	-400	+0	+468	+77	+122	+25	+486

Consistency

PARIS Δρ from JEFF-3.1.1 to BRC-09

Nuclear data	k_{eff}	σ (pcm)	Δk_{eff} (pcm)	σ
JEFF-3.1.1	1,00451	2		
JEFF-3.1.1 + ^{235}U ^{238}U BRC-09	1,00985	2	+534	3
JEFF-3.1.1 + ^{235}U BRC-09	1,00956	2	+505	3
JEFF-3.1.1 + ^{238}U BRC-09	1,00470	2	+19	3
JEFF-3.1.1 + ν ^{235}U BRC-09	1,00393	2	-58	3
JEFF-3.1.1 + ν ^{238}U BRC-09	1,00099	2	-352	3

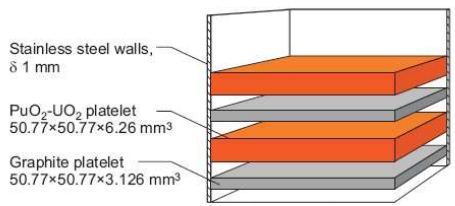
TRIPOLI4 Δρ from JEFF-3.1.1 to BRC-09

Inconsistency : ECCO processing error with MT=5 in BRC-09 eval file

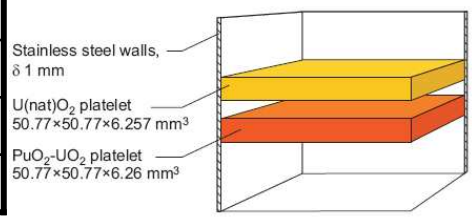
SNEAK 7 analysis

Identical effects for SNEAK 7A, 7B and ZPPR 10A
^{238}U global 7A : -122 vs -66 (13) 7B : -255 vs +4 (12)

7A



7B



Isotope	(n, γ)	ν	(n, f)	(n, n) σ_{el}	(n, n') σ_{inel}	Total
^{238}U	- 22	-397	+258	+68	+13	-122
^{239}Pu	-143	+431	12	-5	-1 (2)	+296
Total						+134

PARIS/SNATCH P1

Isotope	(n, γ)	ν	(n, f)	(n, n) σ_{el}	Total
^{238}U	+257 (2)	-379 (12)	+255 (2)	-195 (3)	-66 (13)
^{239}Pu	-141 (1)	x	+15 (2)	-4 (2)	+305 (13)
Total					+180 (13)

TRIPOLI-4

Because of MT=5 in ^{238}U, PARIS results are inconsistent with TRIPOLI-4 (and MCNP also) ones
⇒ but perturbation calculations very consistent for ^{239}Pu, ^{235}U

Outlook and conclusion

Outlook

- Improvements are needed for **simulation codes**

  Pointwise perturbation calculation from two PENDF files for TRIPOLI-4
  + probability tables treatment

  Calculation time

  σ and μ perturbation calculation for elastic diffusion consistency

- Sensitivities calculation with Monte Carlo (already done « by hand »)

  Automatic parallelization on massively parallel machines (TGCC in France)

- All reactions treated by Monte Carlo codes

  (n, n') reactions : all levels (replacement in evaluation file and new processing)

Outlook

- Development of a toolbox for evaluators based on perturbations analysis

Evaluation files and complete code **libraries DataBase**

Benchmarks (ICSBEP, IRPHE, SINBAD, CEA) **DataBase**

Automatic « intelligent » **processing** (ECCO, TRIPOLI and other codes)

Client/Server technology : produced librairies stored on dedicated server

Global and individual (isotope, reaction, group, anisotropy order …) **neutronic effect calculation** produced by evaluation change : deterministic and stochastic calculations

Different **parameters** : k_{eff}, $\Delta\rho_{Na}$, $\Delta\rho_{T}$, β_{eff}, power density, …

Conclusion

Conclusion

Deterministic and stochastic perturbation methods are of first importance in evaluation effect analysis

Quantification of the effect of the changes between two libraries

Helpful method in processing validation (very important)

Stochastic (long) calculations can be used when deterministic calculation schemes miss or deterministic codes can't answer (anisotropy and heterogeneous geometries for ECCO) → but very long

Consistency between PARIS and TRIPOLI-4

New tools (automatic) for evaluators to automatically check a new evaluation file

Thank you for your attention

Commissariat à l'énergie atomique et aux énergies alternatives
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