

Impact of nuclear data library uncertainties in MYRRHA v1.8 with SUMMON. Library intercomparison

Covariance library intercomparison – JEFF-3.3, ENDF/B-VIII.0 and JENDL-4.0

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- **SUMMON** – S/U analysis code developed at CIEMAT
- MYRRHA
- Uncertainty results in MYRRHA - criticality:
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- Conclusions

SUMMON: Sensitivity and Uncertainty Methodology for MONte carlo codes.

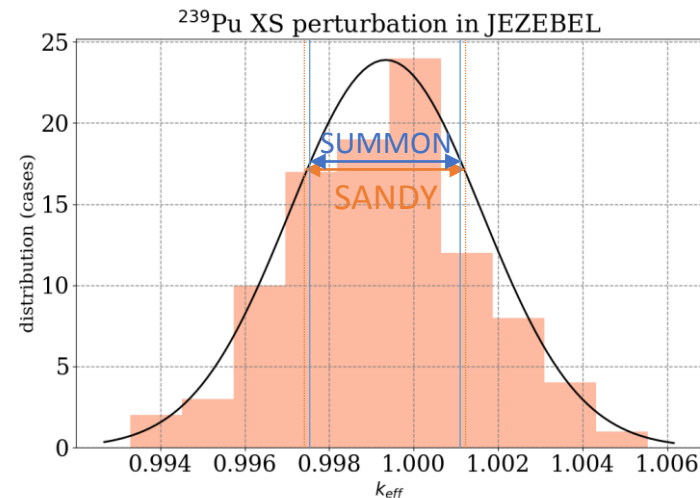
- Flexible tool that can be combined with several Monte Carlo codes and nuclear data libraries
- Deterministic methodology. First-order (linear) propagation of the uncertainty - “sandwich rule”

$$s_{i,\alpha} = \left(\frac{\alpha_1}{i} \frac{\partial i}{\partial \alpha_1}, \dots, \frac{\alpha_k}{i} \frac{\partial i}{\partial \alpha_k} \right)$$

$$var(k) = \sum_{i,j;\alpha\beta} s_{i,\alpha}^T C_{ij;\alpha\beta} s_{j,\beta}$$

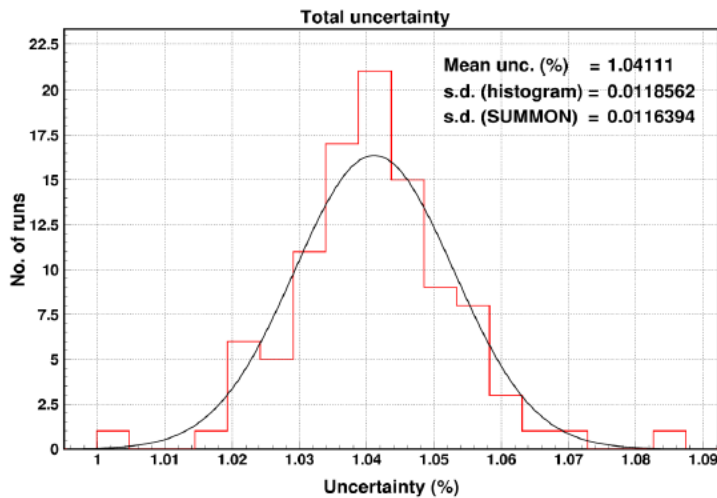
- Verification* with SANDY (stochastic methodology) developed by SCK:

* S. Panizo, et al. Propagation of uncertainty due to nuclear data: stochastic vs. first-order approach. M&C 2023. Accepted.



Statistical uncertainties: sensitivity profiles calculated with MC codes are influenced by statistical errors.

Therefore, the variance due to nuclear data calculated with the sandwich rule is also affected by the statistical uncertainty.



*V. Bécares et al. Progress in neutronic sensitivity and uncertainty analyses at CIEMAT. 47 Annual Meeting of the Spanish Nuclear Society. 2022.

$$var(k) = \sum_{i,j;\alpha\beta} s_{i,\alpha}^T C_{ij;\alpha\beta} s_{j,\beta}$$

$$\sigma^2(var(k)) = \sum_{k;\gamma} \left(\frac{\partial(\sum_{i,j;\alpha\beta} s_{i,\alpha}^T C_{ij;\alpha\beta} s_{j,\beta})}{\partial s_{k,\gamma}} ds_{k,\gamma} \right)^2$$

$$s.d.(k) = \frac{\sigma(var(k))}{2\sqrt{var(k)}} = \frac{\sqrt{\sum_{\beta} (\sum_{\alpha} s_{i,\alpha}^T C_{ij;\alpha\beta} ds_{j,\beta})^2}}{\sqrt{\sum_{\alpha,\beta} s_{i,\alpha}^T C_{ij;\alpha\beta} s_{j,\beta}}}$$

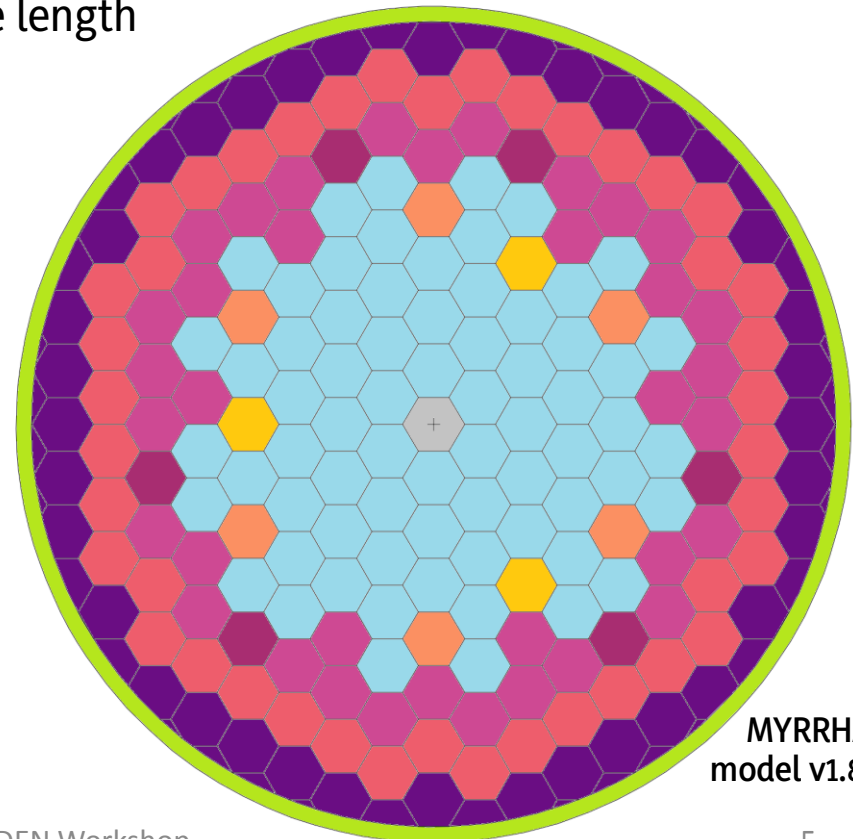
- **MYRRHA**. (Multi-purpose HYbrid Research Reactor for High-tech Applications) is an up to 70 MWth, LBE-cooled fast reactor with both critical and subcritical modes of operation (in the second case, coupled to an accelerator-driven spallation source).
- In this work, version 1.8 of the critical core at BoL design has been considered:
 - MOX fuel (30wt%) Homogenized at assembly level
 - 69 fuel assemblies of 65cm of active length
 - Highly enriched

k_{eff} result MYRRHA v1.8 with MCNP6.2 :

$$k_{eff} = 1.01542(3)$$

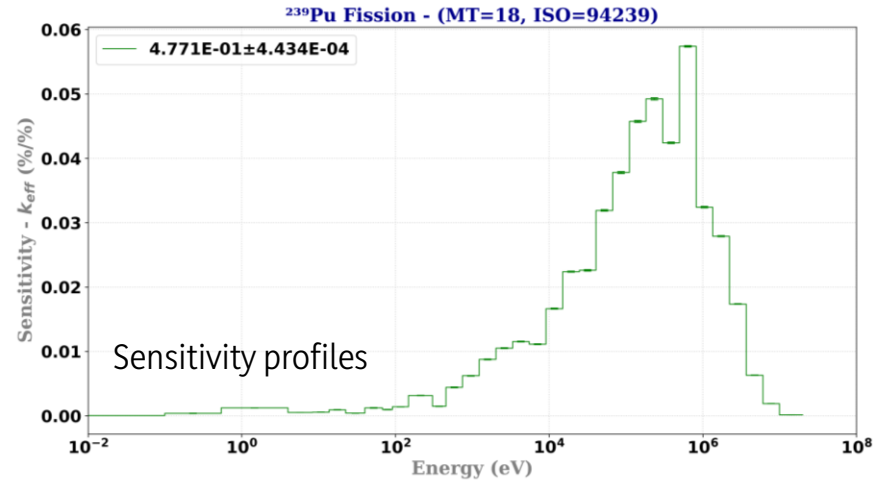
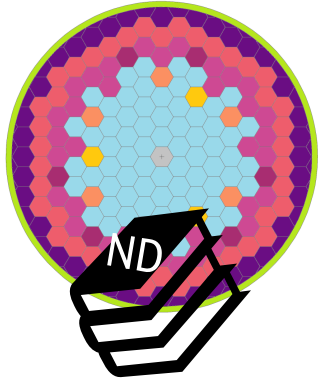
Target accuracy for MYRRHA k_{eff} :

$$TA(k_{eff}) = 300 \text{ pcm}$$



MYRRHA
model v1.8

Methodology – Step by step

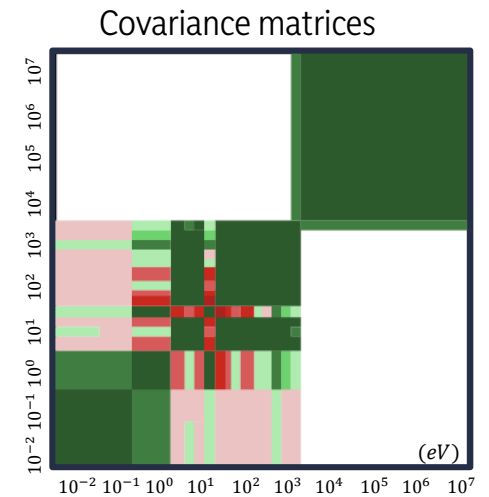
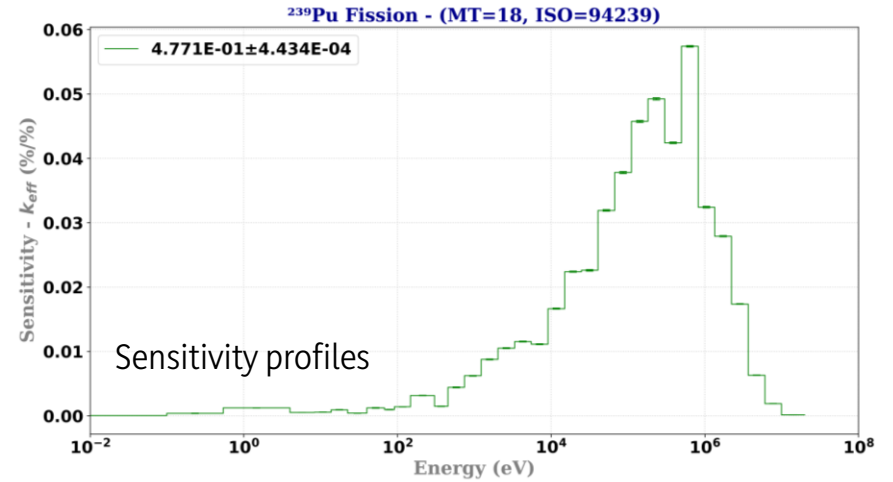
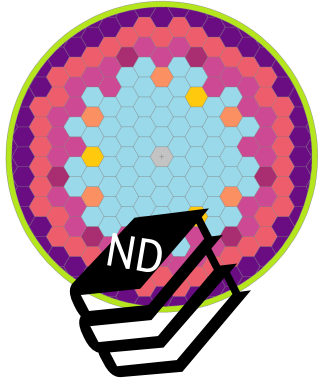


Sensitivity Data File (SDF)

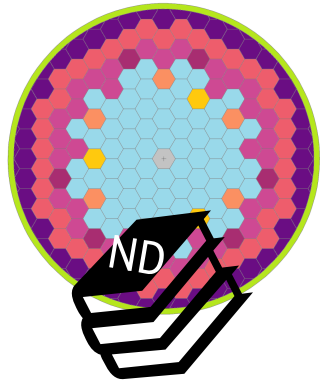
```
./outputfile.io
  33 number of neutron groups
  16946 number of sensitivity profiles          3737 are region integrated
  1.01542 +/- 0.00003 k-eff from the forward case
energy boundaries:
2.000000E+07 1.000000E+07 6.070000E+06 3.680000E+06 2.230000E+06
1.350000E+06 8.210000E+05 4.980000E+05 3.020000E+05 1.830000E+05
1.110000E+05 6.740000E+04 4.090000E+04 2.480000E+04 1.500000E+04
9.120000E+03 5.530000E+03 3.350000E+03 2.030000E+03 1.230000E+03
7.490000E+02 4.540000E+02 3.040000E+02 1.490000E+02 9.170000E+01
6.790000E+01 4.020000E+01 2.260000E+01 1.370000E+01 8.320000E+00
4.000000E+00 5.400000E-01 1.000000E-01 1.000000E-05
1001 elastic 1001 2
  300 0
0.000000E+00 0.000000E+00 0 0
-1.455526E-02 2.538977E-04 1.460757E-02 2.615660E-05 1.054880E-05
1.658100E-06 3.080500E-06 2.141800E-05 -6.835100E-05 -2.075500E-04
-3.678000E-04 -8.300400E-04 -6.984700E-04 -7.493000E-04 -7.298000E-04
-4.808200E-04 -4.895900E-04 -3.875300E-04 -3.473900E-04 -2.616400E-04
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-5.497200E-04 -7.062400E-04 -8.910600E-04 -9.361800E-04 -8.447800E-04
-8.237600E-04 -1.301300E-04 -7.422100E-06
1.402587E-06 3.363290E-06 9.899400E-06 1.384791E-05 2.980418E-05
3.685356E-05 4.233204E-05 6.914853E-05 5.267579E-05 7.816158E-05
8.250871E-05 6.002373E-05 6.541506E-05 6.697679E-05 4.228102E-05
4.895377E-05 4.083916E-05 4.988339E-05 4.716761E-05 5.184179E-05
4.763254E-05 3.539934E-05 4.247488E-05 4.612845E-05 2.743973E-05
3.237851E-05 3.163955E-05 3.296922E-05 2.518324E-05 3.041208E-05
2.553656E-05 1.562861E-05 1.516780E-05
1001 inelastic 1001 4
  300 0
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```

* W. A. Wieselquist, R. A. Lefebvre, Eds., SCALE 6.3.1 User Manual, ORNL/TM-SCALE-6.3.1, UT-Battelle, LLC, Oak Ridge National Laboratory, Oak Ridge, TN (2023).

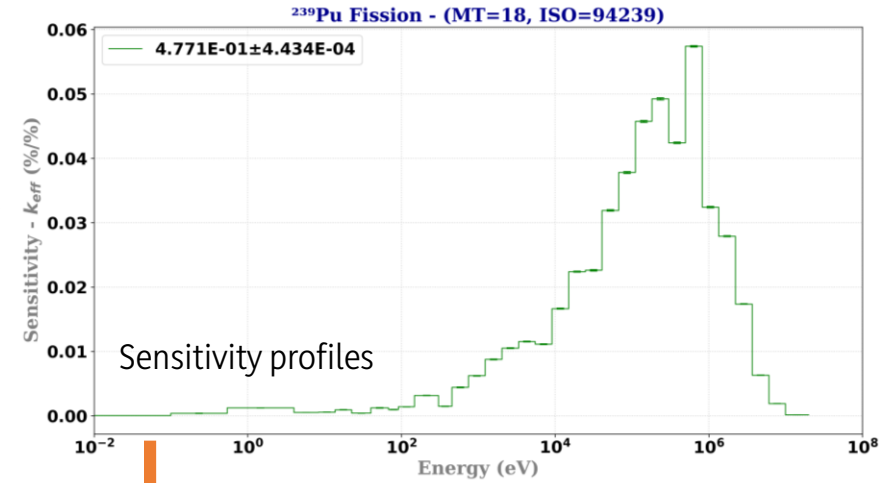
Methodology – Step by step



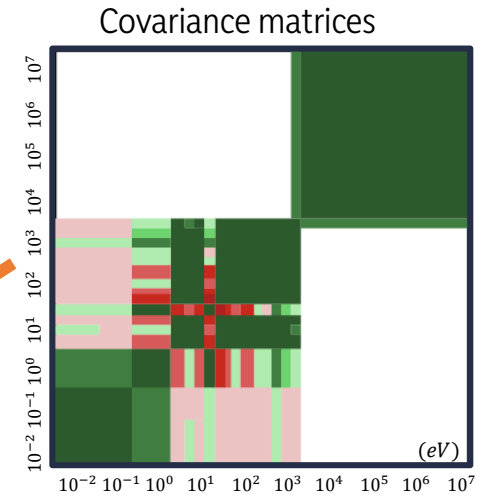
Methodology – Step by step



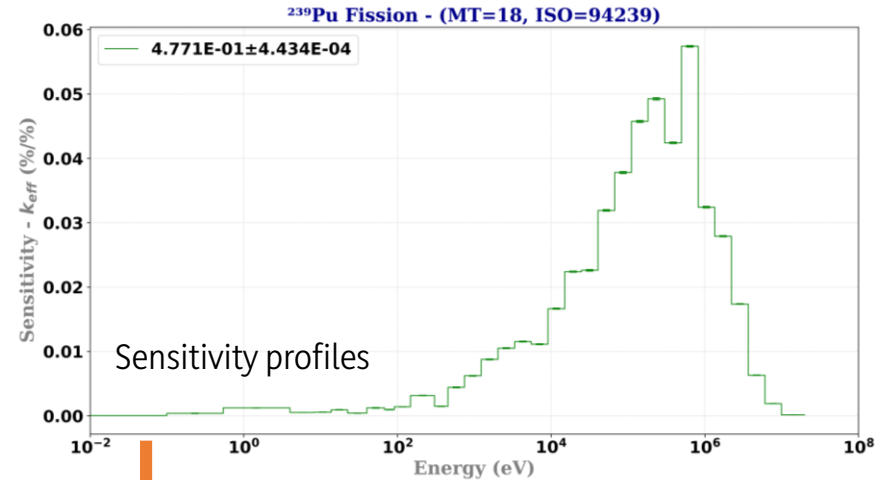
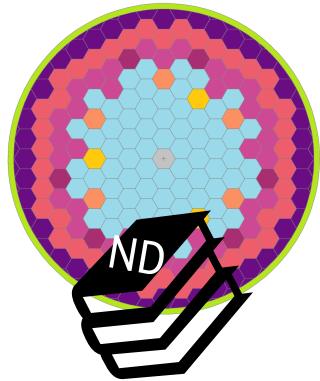
Transport code
MCNP
MONTE CARLO N-PARTICLE



SUM-
+MON

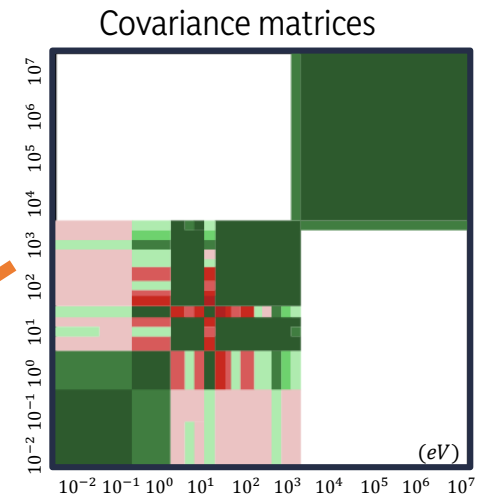


Methodology – Step by step



Quantity	unc (%) ± std MC (%)
²⁴⁰ Pu (n,f) ²⁴⁰ Pu (n,f)	5.54E-01 ± 6.61E-04
²⁴⁰ Pu (n,f) ²⁴⁰ Pu (n,γ)	-4.32E-01 ± 1.72E-04
²³⁹ Pu ν _p ²³⁹ Pu ν _p	3.15E-01 ± 2.03E-04
²³⁹ Pu (n,f) ²³⁹ Pu (n,f)	2.77E-01 ± 3.20E-04
²³⁹ Pu χ ²³⁹ Pu χ	2.37E-01 ± 2.88E-03
Total keff UNC (%)	7.62E-01 ± 1.26E-03

SUM-
+MON



Results – MYRRHA – k_{eff} uncertainties

Table 1

JEFF-3.3

Unc. \pm Stat. Error (%)

^{240}Pu (n,f)	^{240}Pu (n,f)	5.544E-01 \pm 7E-04
^{240}Pu (n,f)	^{240}Pu (n, γ)	-4.316E-01 \pm 2E-04
^{239}Pu v _p	^{239}Pu v _p	3.153E-01 \pm 2E-04
^{239}Pu (n,f)	^{239}Pu (n,f)	2.770E-01 \pm 3E-04
^{239}Pu χ	^{239}Pu χ	2.37E-01 \pm 3E-03
^{240}Pu (n, γ)	^{240}Pu (n, γ)	2.0150E-01 \pm 8E-05
TOTAL keff UNC (%)		7.62E-01 \pm 1E-03

Table 3

ENDF/B-VIII.0

Unc. \pm Stat. Error (%)

^{239}Pu (n,f)	^{239}Pu (n,f)	5.617E-01 \pm 5E-04
^{209}Bi (n,n)	^{209}Bi (n,n)	2.66E-01 \pm 7E-03
^{239}Pu (n, γ)	^{239}Pu (n, γ)	2.207E-01 \pm 2E-04
^{239}Pu v	^{239}Pu v	1.855E-01 \pm 1E-04
^{239}Pu v _p	^{239}Pu v _p	1.851E-01 \pm 1E-04
^{238}U (n, γ)	^{238}U (n, γ)	1.4056E-01 \pm 6E-05
TOTAL keff UNC (%)		7.99E-01 \pm 2E-03

Table 2

JENDL-4.0u

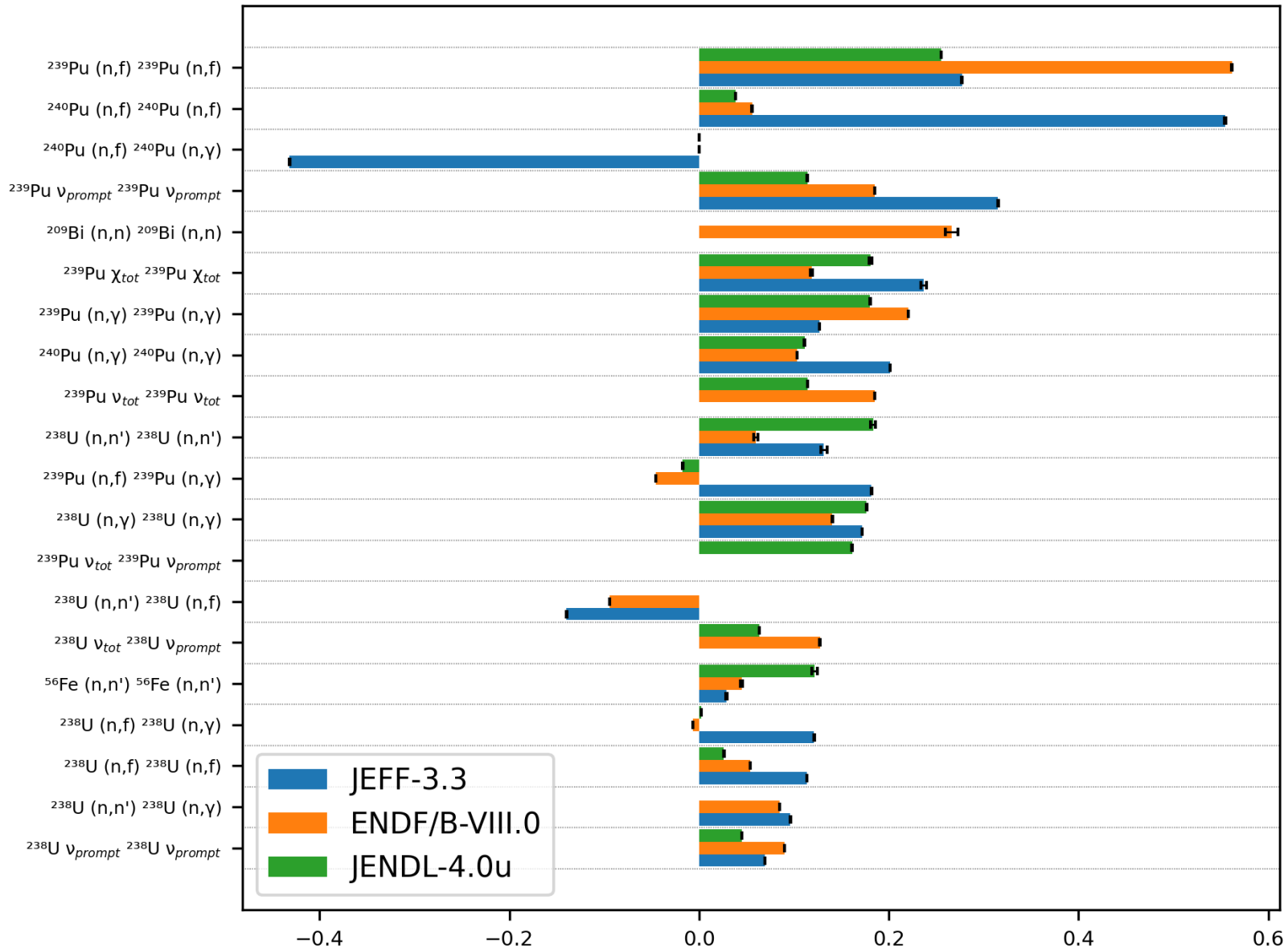
Unc. \pm Stat. Error (%)

^{239}Pu (n,f)	^{239}Pu (n,f)	2.552E-01 \pm 2E-04
^{238}U (n,n')	^{238}U (n,n')	1.84E-01 \pm 3E-03
^{239}Pu χ	^{239}Pu χ	1.81E-01 \pm 2E-03
^{239}Pu (n, γ)	^{239}Pu (n, γ)	1.8041E-01 \pm 9E-05
^{238}U (n, γ)	^{238}U (n, γ)	1.767E-01 \pm 1E-04
^{239}Pu v	^{239}Pu v _p	1.613E-01 \pm 1E-04
TOTAL keff UNC (%)		6.10E-01 \pm 2E-03

Uncertainty due to ND

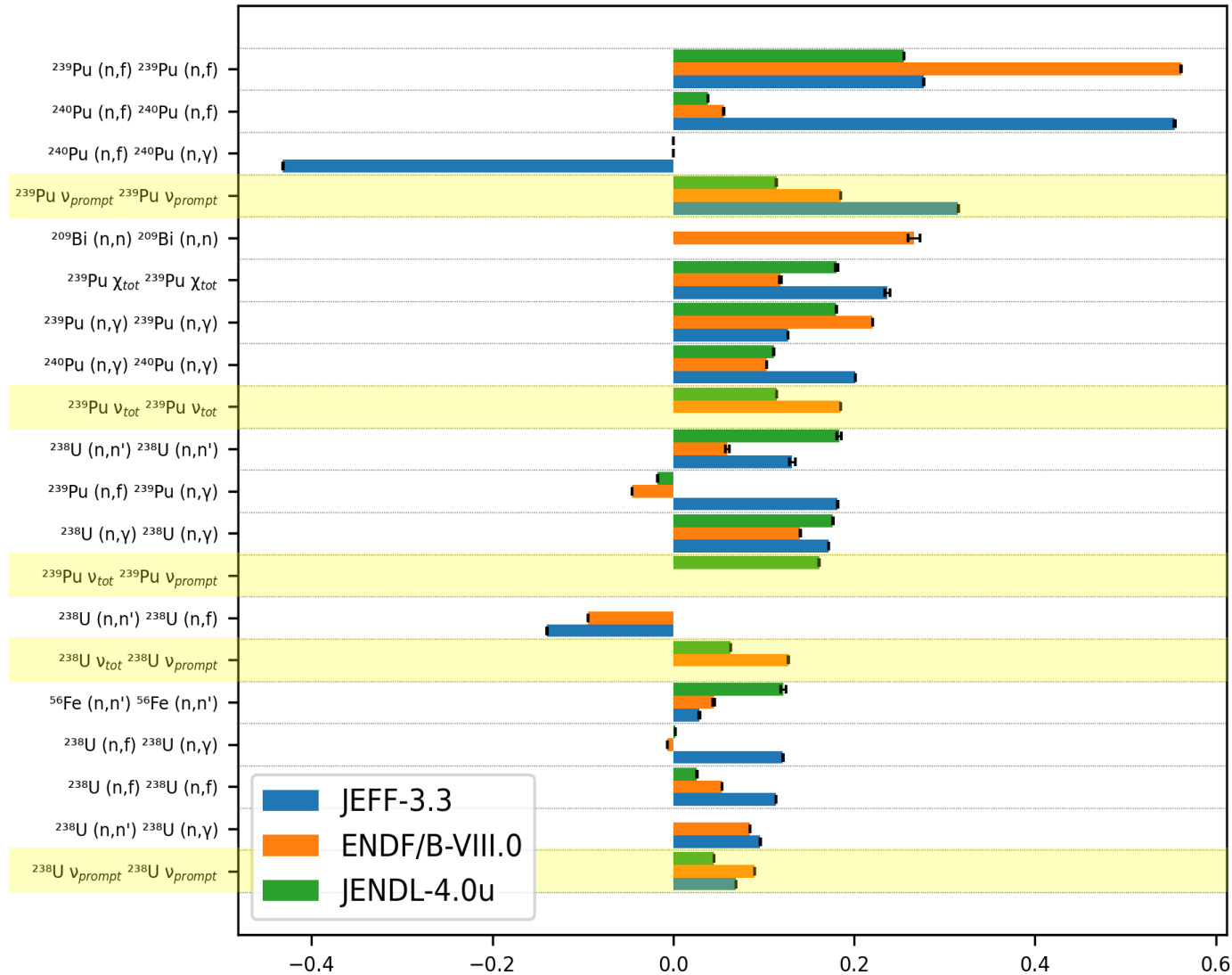
(pcm)	Total	XS Pu239	XS Pu240
JEFF-3.3	774 \pm 1	362.4 \pm 0.3	406.9 \pm 0.9
JENDL 4.0u	619 \pm 2	317.5 \pm 0.2	120.3 \pm 0.2
ENDF/B-VIII.0	811 \pm 2	612.6 \pm 0.7	127.3 \pm 1.3

Results – MYRRHA – k_{eff} uncertainties



Results – MYRRHA – k_{eff} uncertainties - nubar

Since ν and ν_p are two parameters that are strongly correlated, there is the question of whether they should be considered both in uncertainty evaluations or only one should be considered, in order to prevent double-counting.



Results – MYRRHA – k_{eff} uncertainties (MF=31)

Three different situations can be differentiated, according to the covariance information present in the libraries:

Only **covariance information for one parameter** is given (either ν or ν_p).

$^{239}\text{Pu } \nu$

Reaction	JENDL-4.0u	ENDF/B-VIII.0	JEFF-3.3
$\mathbf{V_{total} V_{prompt}}$	0.161	-	-
$\mathbf{V_{total} V_{total}}$	0.114	0.185	-
$\mathbf{V_{prompt} V_{prompt}}$	0.114	0.185	0.315
	0.280	0.262	0.315

If it is ν_p , and considering a single energy group for simplicity, the uncertainty due to it would be:

$$\sigma_1 = \sqrt{s_{\nu_p}^T V s_{\nu_p}} = \sqrt{\frac{\nu_p}{k} \frac{\partial k}{\partial \nu_p} \cdot \frac{Var(\nu_p)}{\nu_p \cdot \nu_p} \cdot \frac{\nu_p}{k} \frac{\partial k}{\partial \nu_p}} = \frac{\sqrt{Var(\nu_p)}}{k} \frac{\partial k}{\partial \nu_p}$$

Results – MYRRHA – k_{eff} uncertainties (MF=31)

Three different situations can be differentiated, according to the covariance information present in the libraries:

In the second case, considering both ν and ν_p in the uncertainty evaluation but not the covariance between them, could result in an overestimation in the total uncertainty by a factor of $\sqrt{2}$, **unless this factor is already taken into account in the covariance evaluation.**

$^{239}\text{Pu } \nu$

Reaction	JENDL-4.0u	ENDF/B-VIII.0	JEFF-3.3
$\mathbf{V_{total} V_{prompt}}$	0.161	-	-
$\mathbf{V_{total} V_{total}}$	0.114	0.185	-
$\mathbf{V_{prompt} V_{prompt}}$	0.114	0.185	0.315
	0.280	0.262	0.315

$$\sigma_2 = \sqrt{s_v^T V s_v} = \sqrt{\begin{pmatrix} \frac{\nu}{k} \frac{\partial k}{\partial \nu} & \frac{\nu_p}{k} \frac{\partial k}{\partial \nu_p} \end{pmatrix} \cdot \begin{pmatrix} \frac{\text{Var}(\nu)}{\nu \cdot \nu} & 0 \\ 0 & \frac{\text{Var}(\nu_p)}{\nu_p \cdot \nu_p} \end{pmatrix} \begin{pmatrix} \frac{\nu}{k} \frac{\partial k}{\partial \nu} \\ \frac{\nu_p}{k} \frac{\partial k}{\partial \nu_p} \end{pmatrix}} \cong \sqrt{2 \frac{\nu}{k} \frac{\partial k}{\partial \nu} \frac{\text{Var}(\nu)}{\nu \cdot \nu} \frac{\nu}{k} \frac{\partial k}{\partial \nu}} = \sqrt{2} \sigma_1$$

Results – MYRRHA – k_{eff} uncertainties (MF=31)

Three different situations can be differentiated, according to the covariance information present in the libraries:

Covariance matrices for all ν , ν_p and cross-correlation between ν and ν_p are included in the library. An overestimation in the total uncertainty by a factor of 2, **unless this factor is already taken into account in the covariance evaluation.**

$^{239}\text{Pu } \nu$

Reaction	JENDL-4.0u	ENDF/B-VIII.0	JEFF-3.3
$\nu_{\text{total}} \nu_{\text{prompt}}$	0.161	-	-
$\nu_{\text{total}} \nu_{\text{total}}$	0.114	0.185	-
$\nu_{\text{prompt}} \nu_{\text{prompt}}$	0.114	0.185	0.315
	0.280	0.262	0.315

$$\sigma_3 = \frac{\sqrt{\text{Var}(k)}}{k} = \sqrt{s_{\nu}^T V s_{\nu}} = \sqrt{\begin{pmatrix} \nu \frac{\partial k}{\partial \nu} & \nu_p \frac{\partial k}{\partial \nu_p} \end{pmatrix} \cdot \begin{pmatrix} \frac{\text{Var}(\nu)}{\nu \cdot \nu} & \frac{\text{Cov}(\nu, \nu_p)}{\nu \cdot \nu_p} \\ \frac{\text{Cov}(\nu, \nu_p)}{\nu \cdot \nu_p} & \frac{\text{Var}(\nu_p)}{\nu_p \cdot \nu_p} \end{pmatrix} \begin{pmatrix} \frac{\nu \partial k}{k \partial \nu} \\ \frac{\nu_p \partial k}{k \partial \nu_p} \end{pmatrix}}$$

Assuming: $\nu \cong \nu_p$, $\partial k / \partial \nu \cong \partial k / \partial \nu_p$ and $\text{Var}(\nu) \cong \text{Var}(\nu_p) \cong \text{Cov}(\nu, \nu_p)$

$$\sigma_3 \cong \sqrt{4 \frac{\nu \partial k}{k \partial \nu} \frac{\text{Var}(\nu)}{\nu \cdot \nu} \frac{\nu \partial k}{k \partial \nu}} = 2 \sqrt{\frac{\nu \partial k}{k \partial \nu} \cdot \frac{\text{Var}(\nu)}{\nu \cdot \nu} \cdot \frac{\nu \partial k}{k \partial \nu}} = 2\sigma_1$$

$^{239}\text{Pu } \nu$			
Reaction	JENDL-4.0u	ENDF/B-VIII.0	JEFF-3.3
$\nu_{\text{total}} \nu_{\text{prompt}}$	0.161	-	-
$\nu_{\text{total}} \nu_{\text{total}}$	0.114	0.185	-
$\nu_{\text{prompt}} \nu_{\text{prompt}}$	0.114	0.185	0.315
	0.280	0.262	0.315

0.161/0.114 $\cong \sqrt{2}$

$^{238}\text{Pu } \nu$			
Reaction	JENDL-4.0u	ENDF/B-VIII.0	JEFF-3.3
$\nu_{\text{total}} \nu_{\text{prompt}}$	0.071	-	0.071
$\nu_{\text{total}} \nu_{\text{total}}$	0.050	0.017	0.050
$\nu_{\text{prompt}} \nu_{\text{prompt}}$	0.050	0.017	0.050
	0.123	0.024	0.123

0.071/0.050 $\cong \sqrt{2}$ *0.071/0.050 $\cong \sqrt{2}$*

$^{238}\text{U } \nu$			
Reaction	JENDL-4.0u	ENDF/B-VIII.0	JEFF-3.3
$\nu_{\text{total}} \nu_{\text{prompt}}$	0.064	0.127	-
$\nu_{\text{total}} \nu_{\text{total}}$	0.045	0.090	-
$\nu_{\text{prompt}} \nu_{\text{prompt}}$	0.045	0.090	0.070
	0.110	0.221	0.070

0.064/0.045 $\cong \sqrt{2}$ *0.127/0.090 $\cong \sqrt{2}$*

- The uncertainties associated with ν_{total} and ν_{prompt} should not be dismissed a priori as redundant, in the cases where the correlation data between them exists. The contribution to the uncertainty could be distributed among the four terms of the covariance matrix.
- Each case must be studied separately. In some cases results are more similar between libraries when all the terms are considered and in other cases they are not.

Conclusions

- **SUMMON** is S/U analysis code with a deterministic methodology that can be combined with several Monte Carlo codes and nuclear data libraries.
- For the k_{eff} in MYRRHA several discrepancies are found between covariance matrices, especially in the following cases:
 - $^{239}\text{Pu}(n,f)$
 - $^{240}\text{Pu}(n,f)$
 - $^{240}\text{Pu}(n,f)$ $^{240}\text{Pu}(n,\gamma)$
 - ^{239}Pu ν and ν_p
 - $^{209}\text{Bi}(n,n)$
- The nubar covariance matrices seems to take into account in the evaluations the existence of total values and should not be discarded a priori.

Thank you for your attention.

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