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WIR SCHAFFEN WISSEN – HEUTE FÜR MORGEN

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Propagation of fission yield uncertainties in CASMO-5 using external sources

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Introduction

Nuclear Data (ND) Uncertainty Quantification (UQ) is made at PSI for a precise bias assessment in:

- Safety Analysis (for application to the SWISS NPP)
- Depletion Analysis (for Burnup Credit, Heat Load)

Fission Yields (FY) have a strong impact on nuclide composition in spent fuel and on the heat load.

The methods for UQ from cross-section uncertainties are well established and the VCM are provided in international evaluations (ENDF/B-VII.1, JEFF-3.2 …). This is not the case of FY

No covariances are available (only variances) for FY. Nevertheless efforts are made to produce them:

- CEA-Cadarache (France)
- ORNL (USA)
- SCK/UPM (Belgium/Spain)
- PSI (Switzerland)

This work aims at:

- Comparing selected (available) FY perturbation methodologies (collaboration with SCK) on a simple case
- Highlight the importance of the covariances: the **uncertainties** but also the **correlations,** for reactor applications

Uncertainty Propagation Platform

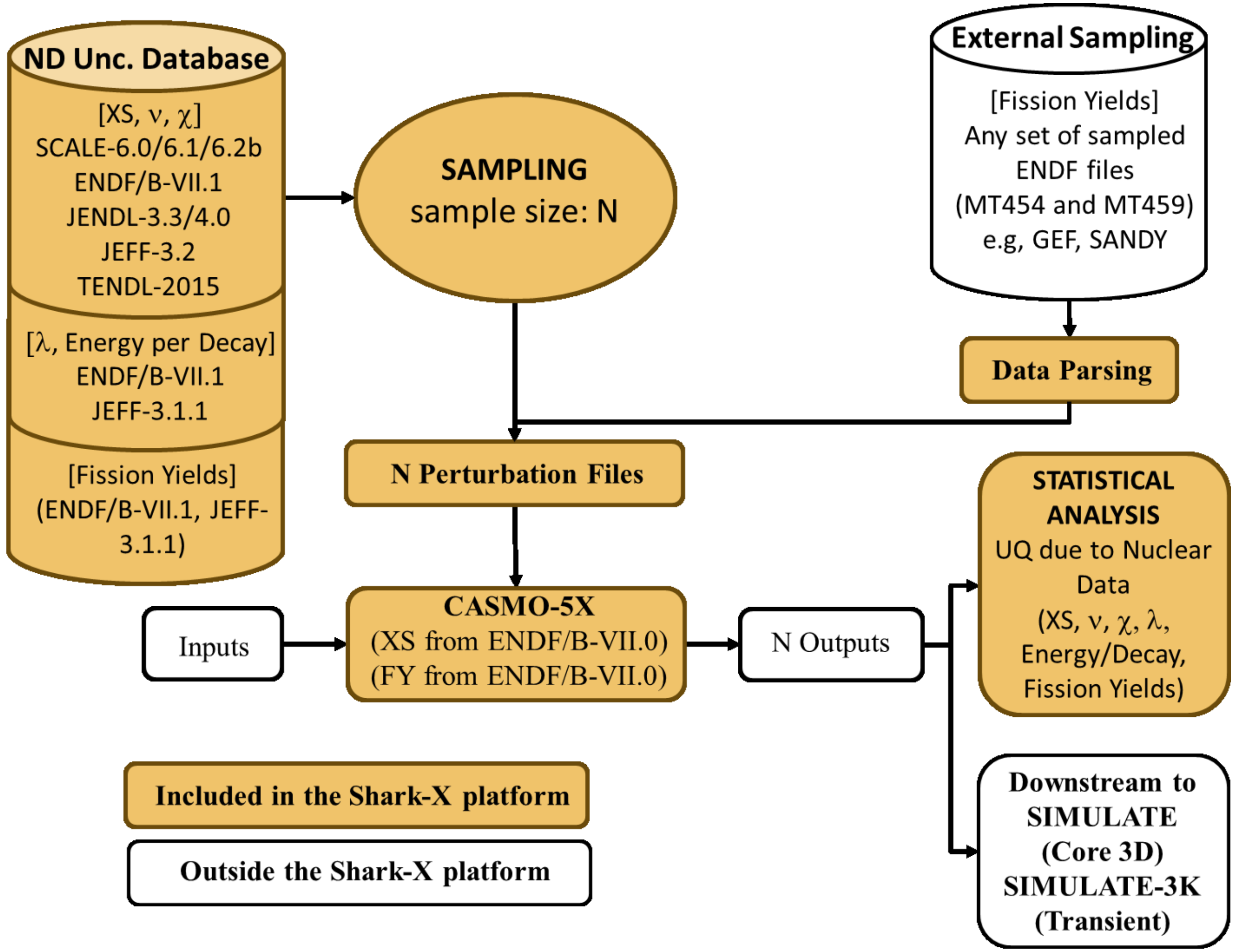
The Shark-X platform includes:

- ND Uncertainty database
- Sampling module
- The CASMO-5 code
- Statistical Analysis module

Capability for Sensitivity Analysis and Uncertainty Quantification using:

- Direct perturbation (sandwich)
- Stochastic Sampling

Shark-X Flowchart for Stochastic Sampling



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Case Description

Perturbations applied on a PWR UO2 fuel assembly [2]

- TMI fuel assembly 4.12w% ^{235}U (density=10.283 g/cm^3)
- 15x15 lattice with 4 Gadolinium pins (2%)
- Burnup up to 60 GWd/MTU
- Calculation with CASMO-5
- 95 Energy Groups for 2D transport solution
- 900 ppm of boron
- Power density: 33,75 W/gU
- **Hot Full Power**

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
2	-	g	-	-	-	-	-	-	-	-	-	-	-	g	-
3	-	-	-	-	-	G	-	-	-	G	-	-	-	-	-
4	-	-	-	G	-	-	-	-	-	-	-	G	-	-	-
5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
6	-	-	G	-	-	G	-	-	-	G	-	-	G	-	-
7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
8	-	-	-	-	-	-	-	I	-	-	-	-	-	-	-
9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
10	-	-	G	-	-	G	-	-	-	G	-	-	G	-	-
11	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
12	-	-	-	G	-	-	-	-	-	-	-	G	-	-	-
13	-	-	-	-	-	G	-	-	-	G	-	-	-	-	-
14	-	g	-	-	-	-	-	-	-	-	-	-	-	g	-
15	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Figure 9: TMI-1 FA Pin Layout

Table 48: TMI-1 FA Pin Descriptions

Marker	Rod Type
g	2.0 weight percent Gd 4.12% ^{235}U pin
G	Guide tube
I	Instrumentation tube
-	4.12% ^{235}U fuel pin

Fission Yield Perturbation

We are considering 4 different methods for the perturbation of the fission yields,
500 samples are created for ^{235}U, ^{239}Pu and ^{241}Pu thermal fission and ^{238}U fast fission for each of the methods

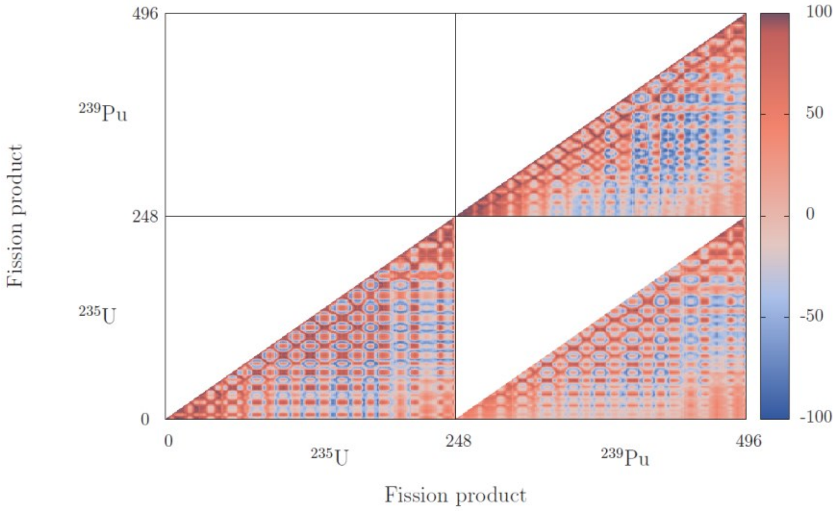
- **GEF** : A General Description of Fission Observables
  - Perturbation of 21 input parameters according to gaussian laws and using the provided GEF uncertainties (Table 7 in [1]).
  - PSI made i.e. different from GEFY-5.3
  - Fulfils the conservation equations

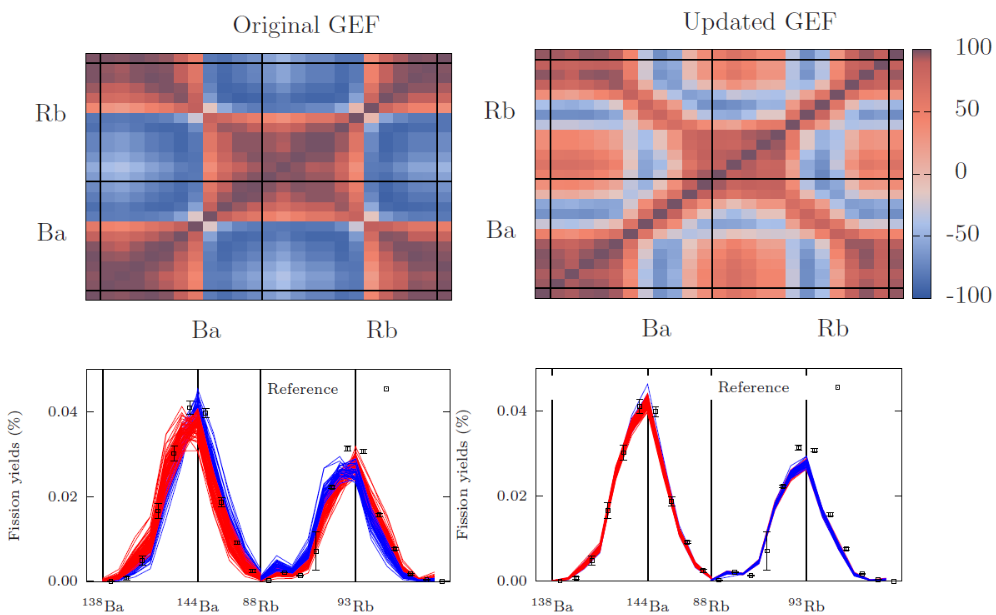
Table 7: Standard deviations of perturbed parameter values

Quantity	σ	unit
Position of the shell for S1 channel	0.1	Z units
Position of the shell for S2 channel	0.1	Z units
Rectangular contribution to the width of S2 channel	0.05	Mass units
Position of the shell for S3 channel	0.1	Z units
Position of the shell at $Z \approx 42$	0.1	Z units
Shell effect at mass symmetry	0.1	MeV
Shell effect for S1 channel	0.1	MeV
Shell effect for S2 channel	0.1	MeV
Shell effect for S3 channel	0.2	MeV
Shell at $Z \approx 42$	0.05	MeV
Curvature of shell for S1 channel	5	%
Curvature of shell for S2 channel	5	%
Curvature of shell for S3 channel	5	%
Curvature of shell at $Z \approx 42$	5	%
$(\hbar\omega)_{eff}$ for tunneling of S1 channel	3	%
$(\hbar\omega)_{eff}$ for tunneling of S2 channel	3	%
$(\hbar\omega)_{eff}$ for tunneling of S3 channel	3	%
$(\hbar\omega)_{eff}$ for tunneling of channel at $Z \approx 42$	3	%
Weakening of the S1 shell with $82/50 - N_{CN}/Z_{CN}$	20	%
Width of the fragment distribution in N/Z	10	%
Charge polarization (Z for fixed A)	0.1	Z units

Fission Yield Perturbation

- **Bayesian Monte Carlo [3]**: Applied to GEF: Same as before with a bayesian feedback to fit the ENDF/B-VII.1 Fission Yields
  - Reduces the uncertainties
  - Changes the correlations
  - Introduces cross-correlations





Fission Yield Perturbation

- **SANDY** : Developed at SCK•CEN it performs Sensitivity Analysis and Uncertainty Quantification of the nuclear data. The covariances between Independent FY (IFY) are created using a Generalized Least Square (GLS) method. The VCM is used to sample the IFY and finally the Cumulative FY (CFY) are obtained by the mean of the Q matrix:

  CFY = Q . IFY

  - Fulfils the conservation equations
  - Reduces the uncertainties (consistency with chain FY uncertainties)
  - Samples performed for ENDF/B-VII.1 and JEFF-3.1.1

- **TENDL-2011** : stochastic sampling on the parameters of the systematics of the fission yields (Wahl), normalization to 2. It has been chosen because the samples are available online
  - No correlation

Comparison to SERPENT

k-inf Uncertainty comparison with SERPENT

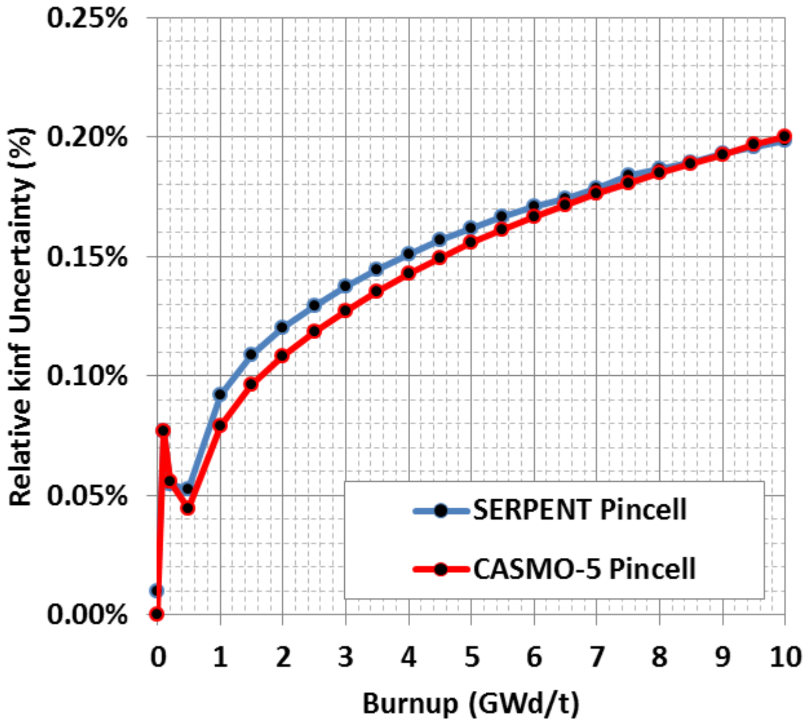
Comparison on a pincell model (based on the lattice)

50 000 neutrons in 500 cycles (+500 hidden cycles)

Doppler-Broadening Rejection Correction (DBRC)

The depletion option used is the Transmutation Trajectory Analysis (TTA): Analytical solution of the linearized chains (idem for CASMO-5)

U^{235} fission yield perturbation (GEF)



Comparison to SERPENT

What is the origin of the peak at low BU ?

A sensitivity analysis between 0 and 1 GWd/tIHM shows the main contributors:

^{135}Xe

^{135}Xe*

^{135}I (decays to ^{135}Xe)

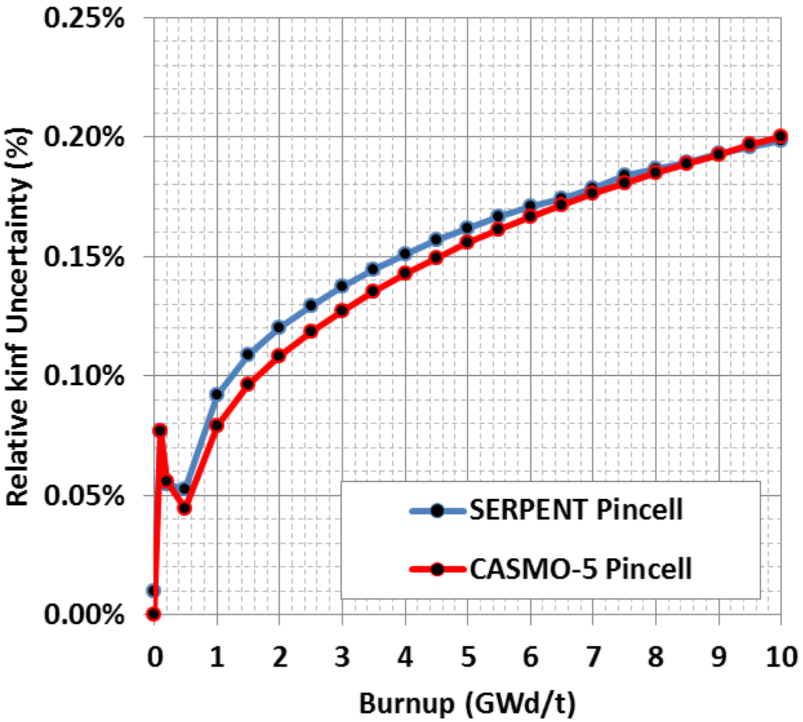
^{149}Nd (decays to ^{149}Pm and ^{149}Sm)

And is **mostly due to the interaction** (i.e. the covariance) between ^{149}Nd and the 3 other isotopes, not directly from the variance !

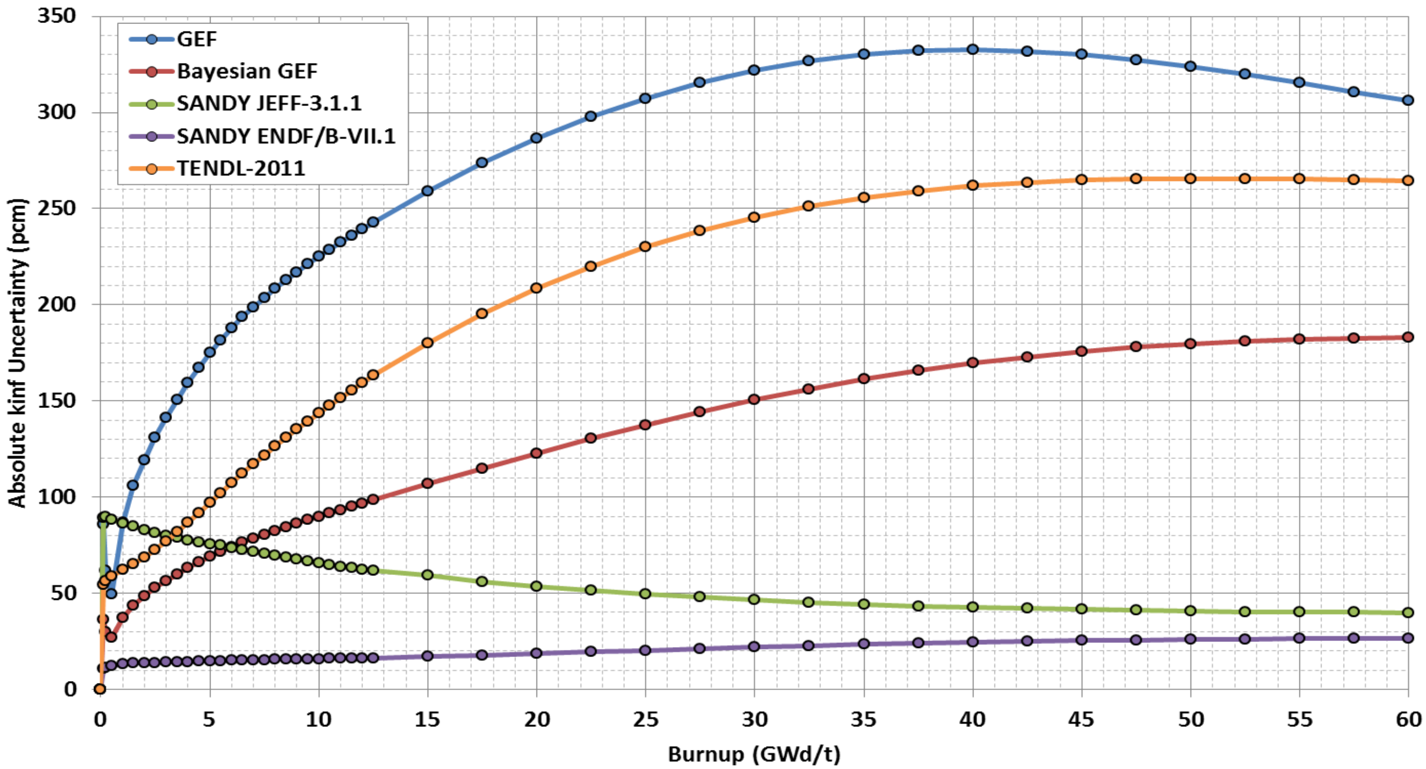
Discrepancy between SERPENT and CASMO-5:

Discrepancy in the transport solution

Different transmutation chains linearization ?



Reactivity Uncertainty



- Different order of magnitude for the kinf uncertainty (no cross-correlations used here)
- The Bayesian feedback ("Bayesian GEF" curve) reduces the kinf uncertainty compared to the GEF method
- The SANDY method creates correlations but also reduces the uncertainty (consistent with chain FY uncertainties) that explains the low uncertainty on kinf

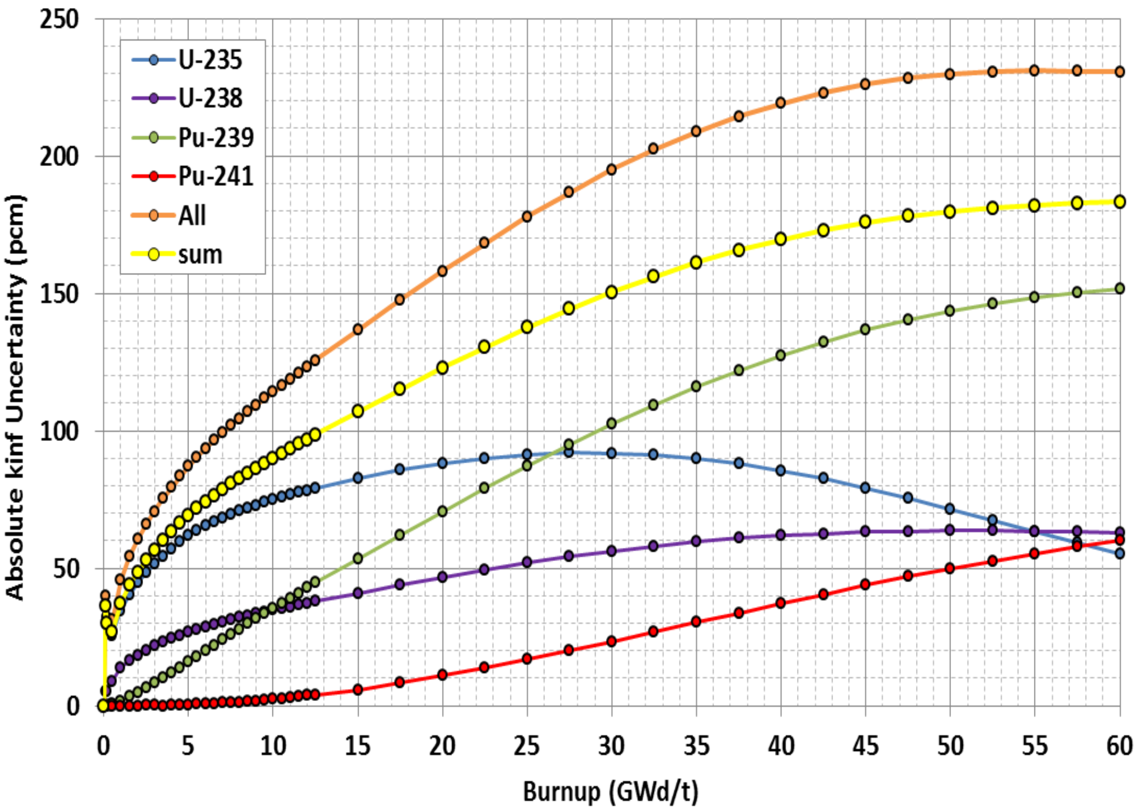
Reactivity Uncertainty

Breakdown according to the four main fathers: ^{235}U, ^{238}U, ^{239}Pu and ^{241}Pu

- Perturbations of the FY from only one father
- Bayesian GEF method

Sum: quadratic sum of the four uncertainties

All: perturbations of all FY, i.e. including cross-correlations (e.g. ^{235}U FY with ^{239}Pu FY)



The cross-correlations increase the total uncertainty, which nevertheless stays lower than the original GEF case

Reactivity Uncertainty

Impact of the branching ratios perturbation:

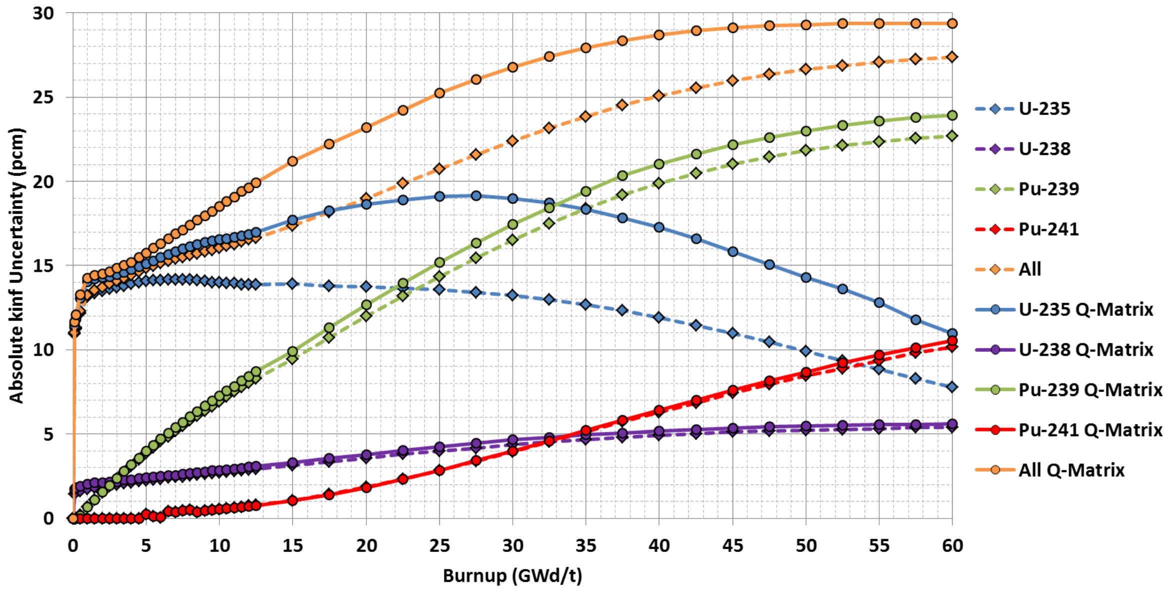
Perturbations of the **branching ratios in the Q matrix** by SANDY

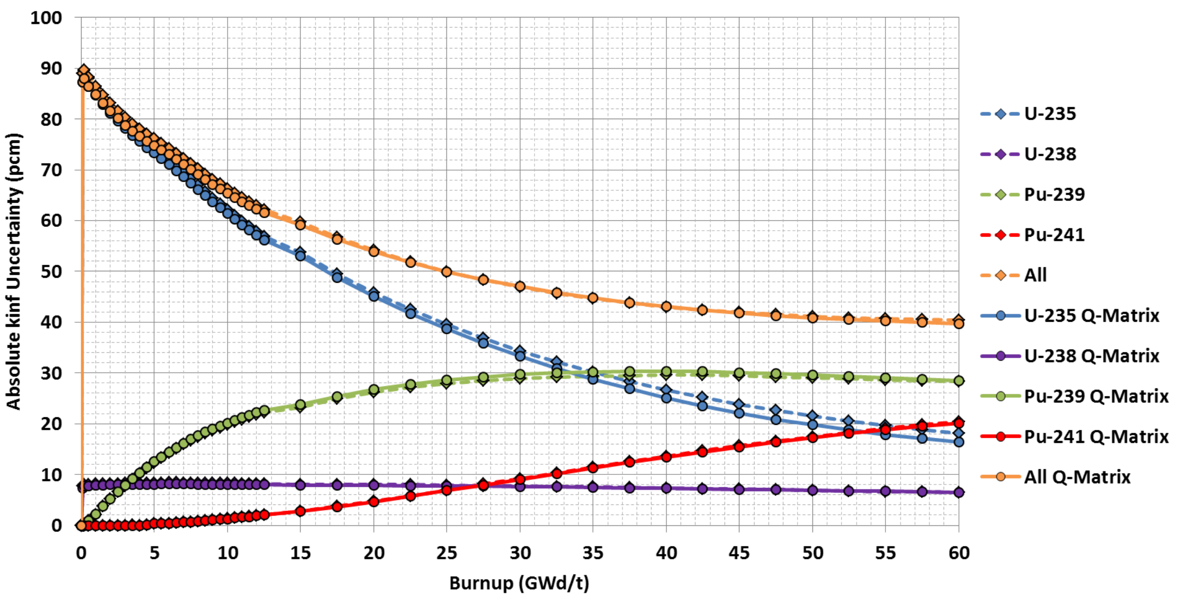
- For ENDF/B-VII.1 (top)

  An effect can be seen for ^{235}U, but the overall uncertainty is very small

- For JEFF-3.1.1 (bottom)
  No noticeable effect !

- Branching ratios in CASMO-5 are not perturbed (only those in the Q-matrix)





Nuclide Composition Uncertainty

- GEF uncertainties are propagated from the fission observable parameters (and are totally independent from the uncertainties stored in evaluations)
- Without correlations, the propagation of TENDL-2011 uncertainties gives rather important uncertainties on some nuclide compositions (^{133}Cs, ^{134}Cs, ^{129}I)
- The effect of the Bayesian feedback is clearly a reduction of the uncertainty for almost all nuclides.
- Unless for few isotopes, the uncertainties found using the SANDY sampling are smaller than those found with the "Bayesian GEF" sampling which highlights the effect of the uncertainty reduction.
- The FY and the chain yields uncertainties are different for ENDF/B-VII.1 and the JEFF-3.1.1. It implies different results using the SANDY code with the two libraries
- JEFF-3.1.1 FY uncertainties lead to generally higher uncertainties

Nuclide	TENDL 2011	GEF	Bayesian GEF	SANDY ENDF/B-VII.1	SANDY JEFF 3.1.1
^{90}Sr	1.34	3.61	2.36	3.58	9.32
^{95}Mo	1.37	3.35	1.78	0.53	0.86
^{99}Tc	1.40	2.62	2.02	3.89	1.05
^{101}Ru	4.62	3.74	1.63	0.68	1.81
^{103}Rh	2.32	6.56	6.66	1.28	2.35
^{109}Ag	36.43	9.89	11.83	8.22	3.44
^{129}I	59.01	11.36	11.50	6.32	6.50
^{131}Xe	2.59	6.38	5.45	3.24	9.28
^{135}Xe	4.18	2.78	2.14	0.50	1.87
^{133}Cs	22.94	4.19	2.58	3.09	3.31
^{134}Cs	22.28	4.18	2.20	2.84	3.35
^{137}Cs	1.51	2.83	1.86	0.31	0.76
^{144}Ce	1.53	3.59	3.04	0.31	0.60
^{142}Nd	1.89	3.17	1.87	0.76	1.59
^{143}Nd	1.39	2.71	2.04	0.44	0.74
^{144}Nd	0.93	3.51	2.05	0.22	0.54
^{145}Nd	1.36	4.70	2.61	0.37	0.82
^{146}Nd	1.25	5.62	2.91	0.63	0.62
^{148}Nd	1.86	8.07	5.37	0.85	0.58
^{147}Sm	1.92	6.98	3.98	0.54	1.08
^{149}Sm	2.20	7.60	7.25	0.46	1.09
^{150}Sm	2.10	8.53	6.04	0.44	1.00
^{151}Sm	2.30	10.36	9.16	0.64	1.57
^{152}Sm	1.95	12.48	10.88	0.58	1.26
^{153}Eu	1.84	13.24	11.11	0.81	1.25
^{154}Eu	1.92	13.87	11.32	0.85	1.23
^{155}Eu	2.19	15.01	12.38	1.00	1.58
^{155}Gd	2.22	15.84	12.62	0.99	1.41
^{156}Gd	2.97	18.57	14.07	1.23	1.72
^{157}Gd	7.08	26.62	19.43	1.42	3.18
^{158}Gd	12.12	37.66	26.14	2.84	3.50

Conclusion

The impact, not only of the **uncertainties** but also of the **correlations** between the fission product yields, on the k-inf and the nuclide composition uncertainties can be strong and depends on the method (GEF)

The effect of the **branching ratios** perturbation is limited for the presented case.
The perturbation itself is also limited in the sense that only branching ratios in the Q-matrix (used to determine the perturbed cumulative FY) are perturbed, not those used by CASMO-5 !

An increase of the uncertainty from the **cross-correlations** (Bayesian GEF method) was shown

Special attention will be paid on the next release of JEFF FY data

A more extensive comparison would be better, using:

- the new release of the GEF perturbed FY (GEFY-5.3)
- the FY covariances from SCALE-6.2
- the FY covariances from CEA-Cadarache

It is planned to extend the study with a decay heat UQ after irradiation

Thank you for your attention !

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References

[1] K-H Schmidt, B. Jurado, C. Amouroux “General Description of Fission Observables GEF Model”, OECD-NEA, JEFF-Report24, (2014)

[2] T. Blyth, N. Porter, M. Avramova, K. Ivanov, E. Royer, E. Sartori, O. Cabellos, H. Ferroukhi and E.Ivanov, "Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation and Safety Analysis of LWRs, Volume II: Specifications and Support Data for the Core Cases (Phase II)," NEA/NSC/DOC(2014), Version 2.0, OECD Nuclear Energy Agency, April,(2014).

[3] D. Rochman, O. Leray, A. Vasiliev, H. Ferroukhi, A.J. Koning, M. Fleming, J.C. Sublet “A Bayesian Monte Carlo method for fission yield covariance information” Submitted to Annals of Nuclear Energy, October 2015