Assessment of nuclear data libraries performance for SFR simulation

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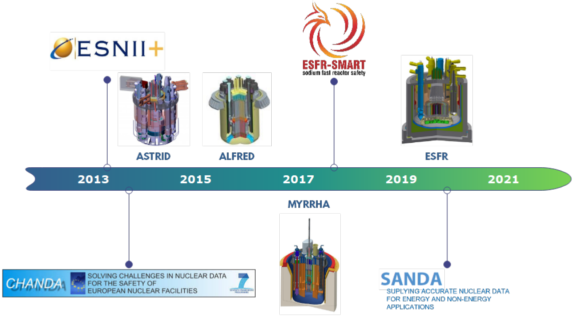
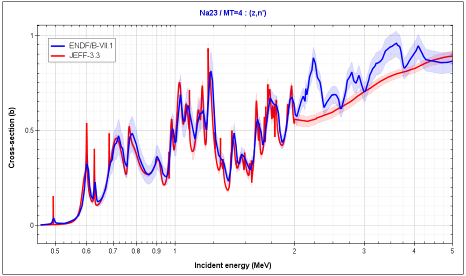
Motivation

- Increasing interest worldwide in Liquid Metal Fast Reactors (LMFR).
- In recent years, UPM has contributed to different European R&D projects that aim to support the design and safety assessment of advanced nuclear systems. This involves the verification and validation (V&V) of computational tools and associated databases.
- Our activities rely on the use of **SCALE Code System** as main computational tool.



Motivation

- **Nuclear data libraries**, as part of the computational scheme, are subject to V&V.
- A reasonable level of knowledge has still not bee reached for all the isotopes and reactions required for fast reactors in spite of several decades of research.
- Then, the use of different nuclear data libraries may lead to very different results, with a different uncertainty quantification.



^{23}Na (n,n') cross section
from JEFF-3.3 and ENDF/B-VII.1.

Motivation

- In the frame of SANDA project, the identification of nuclear data in need of improvement is addressed.
- This will contribute to the production of a more accurate and reliable JEFF-4 library.
- Then, VVUQ activities carried out in this work aim at evaluating the performance of the JEFF-3.3 library for SFR simulation through the systematic use of legacy integral experiments provided by ICSBEP and IRPhEP databases.

SANDA

SANDA

Supplying Accurate Nuclear Data for energy and non-energy Applications

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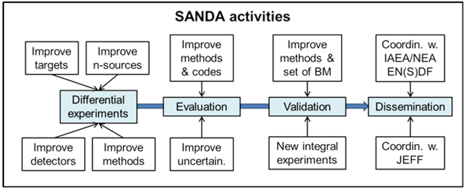

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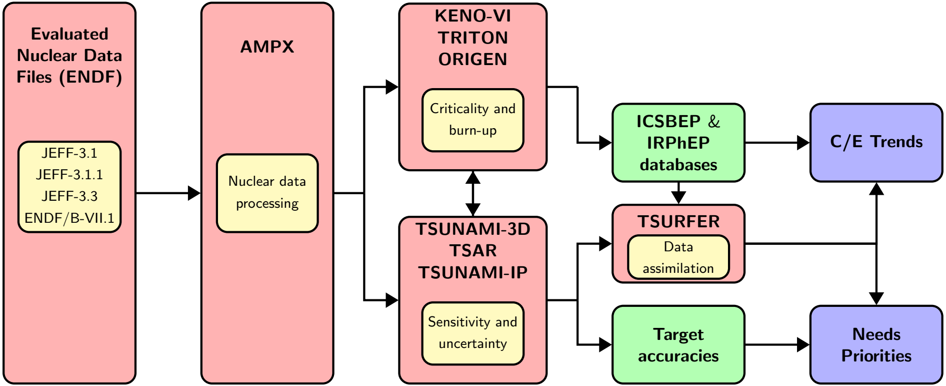
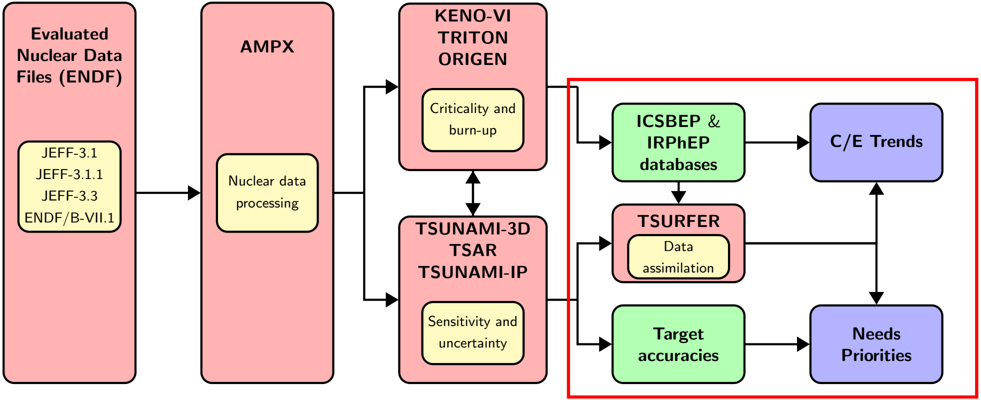
Nuclear data assessment pipeline



A. Jiménez-Carrascosa. "*Methodologies for enhancing the neutronic assessment of Sodium-cooled Fast Reactors: from nuclear data to transient analysis*", **PhD Thesis**, Universidad Politécnica de Madrid, 2023.

Nuclear data assessment pipeline



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- Two different SFR designs are selected, ESFR and ASTRID-like concepts.
- Results from the adjustment are applied to involved evaluated parameters.

Parameter	ESFR	ASTRID-like
Thermal power (MWth)	3600	1500
Coolant	Sodium	Sodium
Fuel type	MOX	MOX
Pu content at inner/outer zone	17.99/17.99	24.3/20.7
Number of SA inner/outer core	216/288	177/114
Core state	EOC	EOC
Evaluated parameters	Multiplication factor Coolant density (full void) Doppler coefficients ($\pm$300 K) Control rod worth	Multiplication factor Coolant density (full void)

Advanced reactor evaluation

- Criticality calculations using KENO-VI
- CE ENDF/B-VII.1 and CE JEFF-3.3 libraries
- Sensitivity analysis using TSUNAMI-3D and TSAR
- Uncertainties via the Sandwich Rule (33-group JEFF-3.3 covariance matrix)

Integral experiments evaluation

- Two different set of experiments, based on ICSBEP and IRPhEP
- Framework supported by available MCNP inputs for IRPhEP benchmarks (sensitivities converted to .sdf format)
- CE JEFF-3.3, CE JEFF-3.1.1 and/or CE ENDF/B-VII.1

Nuclear data assessment for SFR simulation.

Approach: experiment selection

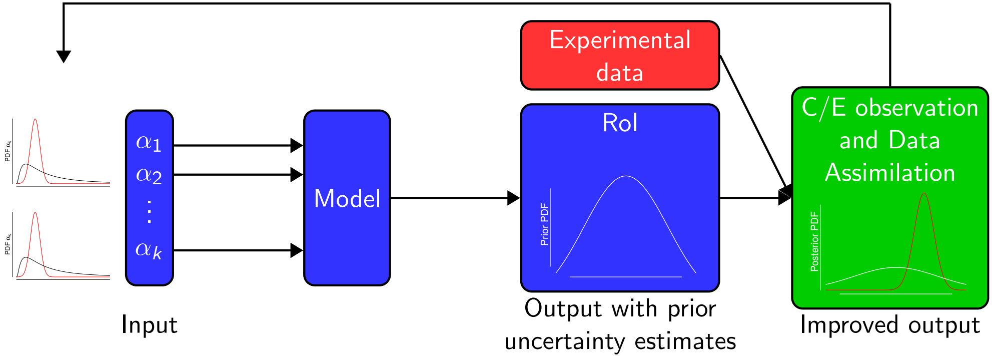
- Experimental databases are set up through the **similarity assessment** (TSUNAMI-IP) with the reference targeted designs:

$$c_k = \frac{S_{R,\alpha}^T V_{\alpha,\alpha} S_{E,\alpha}}{\sqrt{(S_{R,\alpha}^T V_{\alpha,\alpha} S_{R,\alpha})(S_{E,\alpha}^T V_{\alpha,\alpha} S_{E,\alpha})}}$$

- Experimental database selected from IRPhEP targeting not only criticality cases but also sodium void effect, Doppler coefficient and control rod worth.

Nuclear data assessment for SFR simulation
Approach: TSURFER framework

The framework for Data Assimilation is based on the TSURFER code (GLLS methodology).



Information provided by experimental data is transferred to the employed nuclear data library, JEFF-3.3, to improve the model output with constraint uncertainties.

Results for advanced systems: overview

- Impact of different nuclear data libraries on SFR parameters:

Reactor	Response	JEFF-3.3	ENDF/B-VII.1	Difference (pcm)
ESFR	Multiplication factor k_{eff}	1.00378 ± 0.00010	1.00072 ± 0.00010	306
	Sodium void worth ρ_{Na}	500 ± 13	270 ± 14	230
	Doppler effect ρ_T +300 K	-134 ± 14	-121 ± 14	-13
	Doppler effect ρ_T -300 K	167 ± 14		
	Control rod worth ρ_{CR}	-5000 ± 14	-4805 ± 14	-195
ASTRID	Multiplication factor k_{eff}	1.00296 ± 0.00010	0.99936 ± 0.00010	360
	Sodium void worth ρ_{Na}	-375 ± 14	-581 ± 14	206

- JEFF-3.3 results overestimate both multiplication factor and sodium void worth effect compared to ENDF/B-VII.1 values.

Nuclear data assessment for SFR simulation

Results for advanced systems: uncertainty propagation

- Nuclear data uncertainty quantification results using two difference covariance matrices:

Reactor	Response	Uncertainty (%) JEFF-3.3	Uncertainty (%) ENDF/B-VIII.0	Target accuracy (%)
ESFR	k_{eff}	**1.036 ± 2.6E-04**	**0.904 ± 1.0E-04**	0.3
	ρ_{Na}	**15.68 ± 7.6E-02**	**20.45 ± 8.2E-02**	7
	ρ_T +300 K	4.41 ± 5.7E-01	3.75 ± 6.7E-01	7
	ρ_T -300 K	4.21 ± 5.5E-01	3.94 ± 7.6E-01	7
	ρ_{CR}	1.97 ± 1.1E-02	1.58 ± 9.8E-03	7
ASTRID	k_{eff}	**0.970 ± 2.0E-04**	**0.891 ± 5.4E-05**	0.3
	ρ_{Na}	**22.55 ± 7.4E-02**	**26.27 ± 4.9E-02**	7

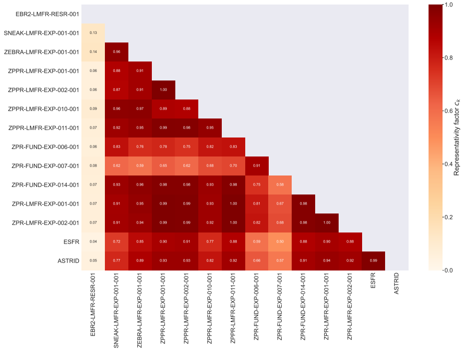
Target accuracies exceeded for k_{eff} and ρ_{Na}

Role of data adjustment techniques.

Nuclear data assessment for SFR simulation

Experimental database: multiplication factor

Benchmark identifier in IRPhEP	Fuel/Other	Experimental facility	Institution
EBR2-LMFR-RESR-001	UO_2/Sodium	EBR-II	ANL, USA
SNEAK-LMFR-EXP-001	MOX/Sodium	SNEAK 7A	KFK, Germany
ZEBRA-LMFR-EXP-001	Pu metal-UO_2/Sodium	ZEBRA 22	AEEW, UK
ZPPR-LMFR-EXP-001	MOX/Sodium	ZPPR-10A	ANL, USA
ZPPR-LMFR-EXP-002	MOX/Sodium	ZPPR-9	ANL, USA
ZPPR-LMFR-EXP-010	MOX/Sodium	ZPPR-12	ANL, USA
ZPPR-LMFR-EXP-011	MOX/Sodium	ZPPR-2	ANL, USA
ZPR-FUND-EXP-006	Pu-U alloys/Graphite	ZPR-3/53	ANL, USA
ZPR-FUND-EXP-007	Pu-U alloys/Graphite	ZPR-3/54	ANL, USA
ZPR-FUND-EXP-014	Pu-U carbide/Sodium	ZPR-9/31	ANL, USA
ZPR-LMFR-EXP-001	MOX/Sodium	ZPR-6/7	ANL, USA
ZPR-LMFR-EXP-002	MOX/Sodium	ZPR-6/7	ANL, USA

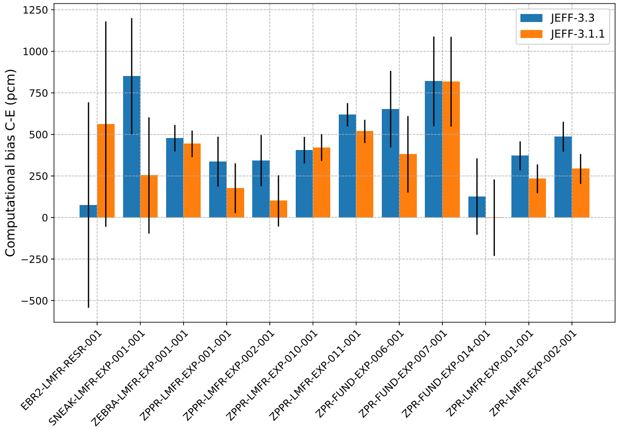


Similarity matrix.

Nuclear data assessment for SFR simulation

Experimental database: criticality

- These experiments are evaluated using two different nuclear data libraries:



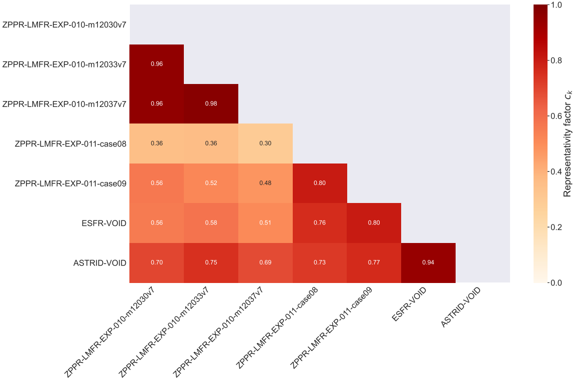
- Average C-E deviation of 463 pcm for JEFF-3.3 results, while JEFF-3.1.1 performs slightly better.
- In general, JEFF-3.3 results systematically overestimate experimental values.
- The main sources of discrepancies are identified:
  - $^{238}\mathrm{U}$ (n,γ)
  - $^{239}\mathrm{Pu}$ $\bar{\nu}$
  - $^{239}\mathrm{Pu}$ (n,f)
  - $^{239}\mathrm{Pu}$ χ
  - $^{23}\mathrm{Na}$ (n,n')

Nuclear data assessment for SFR simulation

Experimental database: sodium void worth

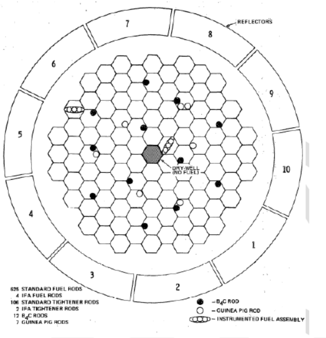
Experiments with large sodium void worth values are particularly selected:

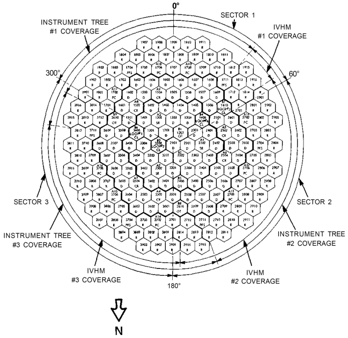
Benchmark identifier	Experimental facility	Core Loading
ZPPR-LMFR-EXP-010-m12030	ZPPR-12	Loading 30
ZPPR-LMFR-EXP-010-m12033	ZPPR-12	Loading 33
ZPPR-LMFR-EXP-010-m12037	ZPPR-12	Loading 37
ZPPR-LMFR-EXP-011-case08	ZPPR-2	Loading 184
ZPPR-LMFR-EXP-011-case09	ZPPR-2	Loading 185



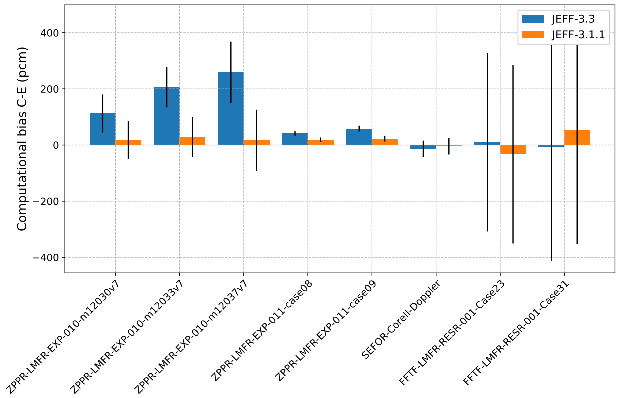
The following experiments are selected targeting Doppler effect and control rod worth:

- There is a lack of experiments in the IRPhEP database regarding Doppler measurements → SEFOR experiments selected.
- A variety of control rod worth measurements is provided by the FFTF experiment → Two configurations selected.





- These reactivity experiments are evaluated using two different nuclear data libraries:

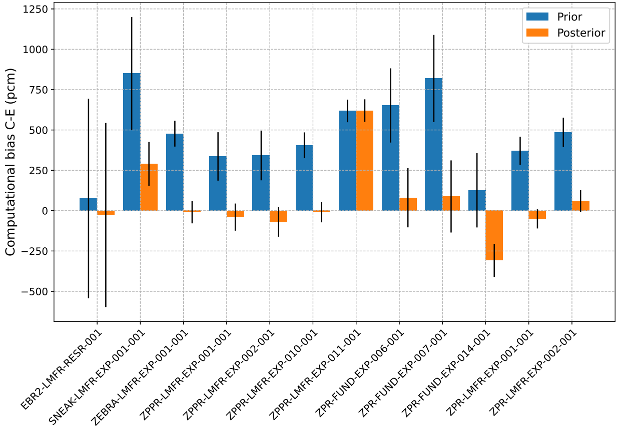


- Again, JEFF-3.3 systematically overestimate the experimental results concerning the sodium void reactivity effect.
- The main sources of discrepancies are again identified:
  - ^{23}Na (n,n)
  - ^{23}Na (n,n')
  - ^{239}Pu (n,f)
  - ^{239}Pu (n,γ)
  - ^{23}Na (n,γ)
- Negligible deviations are observed for Doppler effect.
- JEFF-3.3 results show an excellent agreement with FFTF benchmark values, with discrepancies lower than 10 pcm.

- The established experimental database is applied with the aim of improving JEFF-3.3 results.
- Experiments might be omitted through the chi-filtering in TSURFER.
- The following information is required before performing the adjustment:
  - Prior JEFF-3.3 nuclear data covariance matrix,
  - Sensitivity profiles for every experiment-response,
  - Active responses: experiment benchmarks,
  - Passive responses: target SFR designs under analysis,
  - Experiment covariance data: **scarcely available!** Conservative correlations are assumed.
- As a result, a set of MG adjusted cross section and covariance data set is obtained.

Nuclear data assessment for SFR simulation

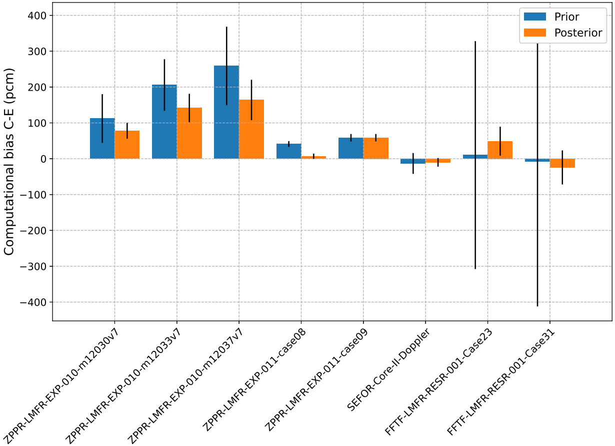
Data Assimilation: results



- Post-assimilation results reduce the computational bias from 463 to 127 pcm concerning criticality database, obtaining a better agreement for most of experiment benchmarks.
- Simultaneously, TSURFER is able to provide a quality adjustment for reactivity effects, even though they might be reversed.

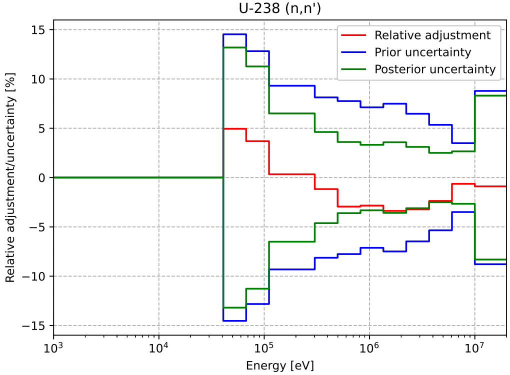
Nuclear data assessment for SFR simulation

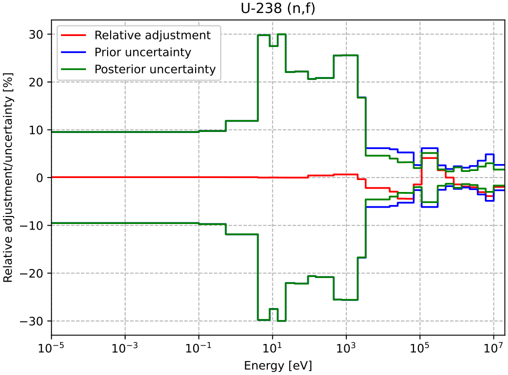
Data Assimilation: results



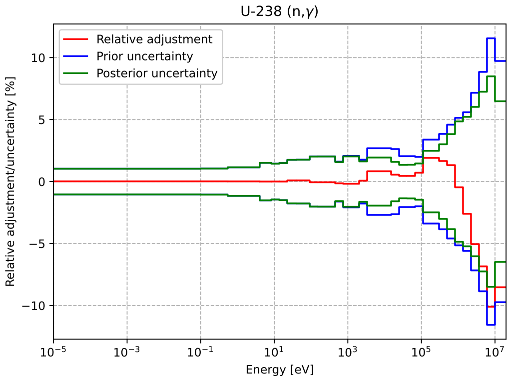
- The *C*/*E* discrepancy of sodium void effect is slightly reduced by around 35% for ZPPR-LMFR-EXP-010 cases.
- When involving sodium void reactivity effects to the adjustment, $^{239}\mathrm{Pu}\ \chi$ and $^{238}\mathrm{U}$ major cross sections become the more relevant quantities to be adjusted.

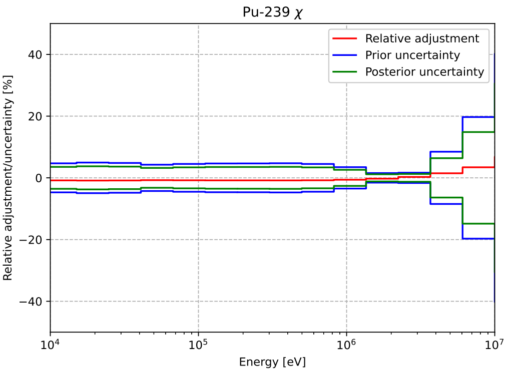
- Major adjustments:





- Major adjustments:





- As a result of the adjustment, ESFR and ASTRID main responses will be impacted as follows:

Reactor	Response	JEFF-3.3 prior	JEFF-3.3 posterior	Bias (pcm)
ESFR	Multiplication factor k_{eff}	1.00378 $\pm$ 0.00010	1.00130	-250
	Sodium void worth ρ_{Na}	500 $\pm$ 13	450	-50
	Doppler effect ρ_T +300 K	-134 $\pm$ 14	-136	-2
	Doppler effect ρ_T -300 K	167 $\pm$ 14	164	-3
	Control rod worth ρ_{CR}	-5000 $\pm$ 14	-5064	-64
ASTRID	Multiplication factor k_{eff}	1.00296 $\pm$ 0.00010	1.00040	-260
	Sodium void worth ρ_{Na}	-375 $\pm$ 14	-443	-68

- Results are consistent with derived trends associated to representative experiments.
- k_{eff} results mostly improve due to ^{238}U (n,n'), ^{238}U (n,f), ^{238}U (n,γ) and ^{239}Pu $\bar{\nu}$ adjustments.
- ρ_{Na} values mostly improve due to ^{239}Pu (n,f) and ^{56}Fe (n,n) changes.

- Adjusted nuclear data also provide constrained uncertainties, allowing to reevaluate the nuclear data-induced uncertainty in ESFR and ASTRID parameters:

Reactor	Response	Uncertainty (%) JEFF-3.3 Prior	Uncertainty (%) JEFF-3.3 Posterior
ESFR	k_{eff}	1.036	0.306
	ρ_{Na}	15.68	7.71
	ρ_T +300 K	4.41	2.56
	ρ_T -300 K	4.21	3.10
	ρ_{CR}	1.97	1.12
ASTRID	k_{eff}	0.970	0.249
	ρ_{Na}	22.55	10.02

- Strong uncertainty reductions are obtained, bringing k_{eff} uncertainty close or below the target accuracy.
- This is mainly due to new cross-correlations appearing in the posterior covariance matrix.

- The posterior uncertainty breakdown points out this observation:

Prior ESFR k_{eff}		Posterior ESFR k_{eff}	
Quantity	$\Delta k_{eff}/k_{eff}$ (%)	Quantity	$\Delta k_{eff}/k_{eff}$ (%)
^{240}Pu (n,f) - ^{240}Pu (n,f)	0.584	^{240}Pu (n,f) - ^{240}Pu (n,f)	0.423
^{238}U (n,n') - ^{238}U (n,n')	0.475	^{240}Pu (n,f) - ^{240}Pu (n,γ)	-0.326
^{239}Pu χ - ^{239}Pu χ	0.431	^{239}Pu χ - ^{239}Pu χ	0.325
^{240}Pu (n,f) - ^{240}Pu (n,γ)	-0.419	^{238}U (n,γ) - ^{239}Pu χ	-0.260
^{238}U (n,n') - ^{238}U (n,f)	-0.346	^{239}Pu (n,f) - ^{239}Pu (n,f)	0.249
^{239}Pu (n,f) - ^{239}Pu (n,f)	0.316	^{239}Pu $\bar{\nu}$ - ^{239}Pu $\bar{\nu}$	0.245
^{238}U (n,γ) - ^{238}U (n,γ)	0.303	^{239}Pu (n,f) - ^{239}Pu $\bar{\nu}$	-0.229
^{238}U (n,n') - ^{238}U (n,γ)	0.298	^{238}U (n,n') - ^{239}Pu χ	-0.225
^{239}Pu $\bar{\nu}$ - ^{239}Pu $\bar{\nu}$	0.295	^{238}U (n,n') - ^{238}U (n,n')	0.221
^{238}U (n,f) - ^{238}U (n,γ)	0.198	^{238}U (n,γ) - ^{238}U (n,γ)	0.214
TOTAL	1.036	TOTAL	0.306

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Conclusions

- Framework for nuclear data validation targeting SFR analyses: recommendations on related nuclear data needs.
- Integral experiments can play an important role on the nuclear data life cycle in combination with data assimilation techniques.
- This framework allows to evaluate the nuclear data performance for SFR analyses, providing recommendations on related needs and priorities.
- Data adjustment as a key computational approach for nuclear data assessment.

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Future work

- Accurate estimation of correlations in experiment uncertainties.
- Extension of SCALE capabilities to include kinetic parameters.
- Extension of experimental database for more comprehensive adjustment analysis.
- The application of TSURFER for the assessment of the latest JEFF-4T2 library is currently ongoing (lack of crucial covariances: $^{56}\mathrm{Fe}$, $^{239}\mathrm{Pu}$, $^{240}\mathrm{Pu}$)

Thank you for your attention

This work is part of the SANDA project (Supplying Accurate Nuclear Data for energy and non-energy Applications) that has received funding from the European Union's H2020/Euratom under grant agreement No. 847552.