

# Benchmarking, Nuclear Data Validation and Adjustment for fast reactor systems using IRPhEP

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Workshop on Nuclear Databases for Nuclear Reactor Applications  
Universidad Politécnica de Madrid, September 20, 2022

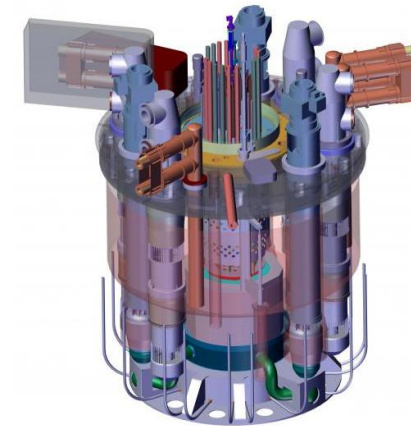


**POLITÉCNICA**

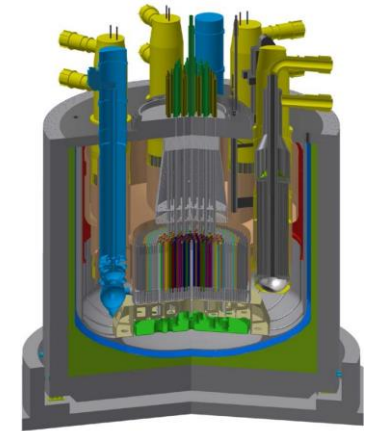
“Ingeniamos el futuro”

# Motivation

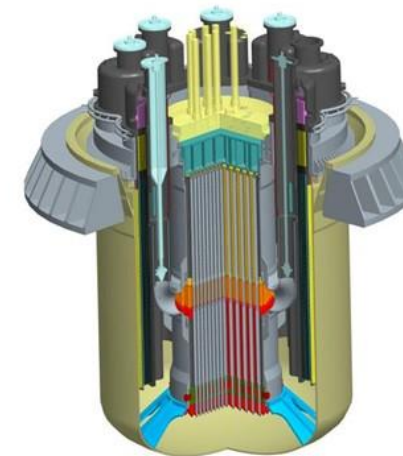
- Increasing interest in liquid metal fast reactors (LMFR)
- In recent years, UPM has participated into different European R&D projects
- ... with a common objective: validate computational approaches to support the development of LMFR
- ... which includes nuclear data, important source of uncertainties in computational outcomes



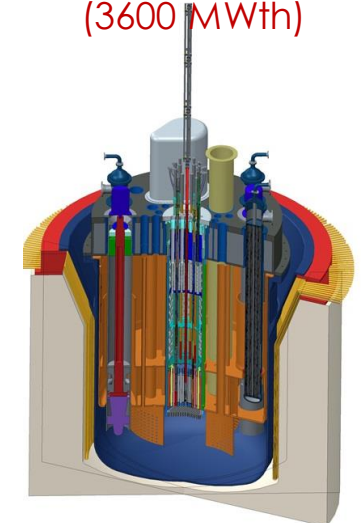
**ASTRID**  
(1500 MWth)



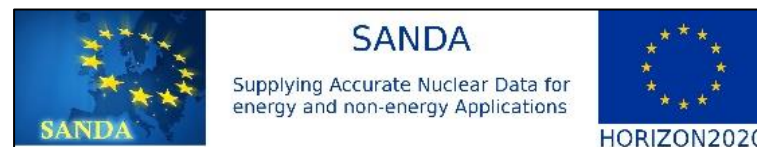
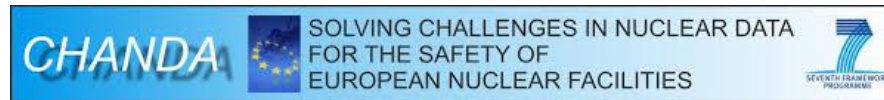
**ESFR**  
(3600 MWth)



**LFR ALFRED**  
(300 MWth)



**LFR MYRRHA**  
(100 MWth)



# Motivation

- The use of different ND libraries for LMFR provides very different results, with a different uncertainty quantification
- **Objective:** to identify the ND in need of improvement to produce an accurate and reliable JEFF library with a view on the next release (JEFF-4.0)
- Legacy reactor physics experiments in the IRPhE Handbook are very valuable

Table 5.1. Nuclear data library effect on BOC k-effective values (pcm)

Calculations	Libraries	Code	MOX-3600	CAR-3600	MET-1000	MOX-1000
ANL-3 - ANL-2	JEFF3.1 - ENDFB7.0	MCNP5	610	869	1232	757
ANL-5 - ANL-4	JEFF3.1 - ENDFB7.0	ERANOS	538	774	1058	646
CEA-5 - CEA-6	JEFF3.1 - ENDFB6.8	ERANOS	-292			
CEA-5 - CEA-7	JEFF3.1 - ENDFB7.0	ERANOS	530			
CEA-5 - CEA-8	JEFF3.1 - ENDFB7.1	ERANOS	503			696
CEA-5 - CEA-9	JEFF3.1 - JENDL4.0	ERANOS	495		808	
CEN-2 - CEN-1	JEFF3.1.2 - ENDFB7.1	MCNPX/ALE PH-2.5				867
UIUC-1 - UIUC-2	JEFF3.1.1 - ENDFB6.8	SERPENT	-568	-650	-191	198
UIUC-1 - UIUC-3	JEFF3.1.1 - ENDFB7.0	SERPENT	391	525	851	561

Reactor	Response	Target accuracy (OECD/NEA WPEC SG46)	Uncertainty [%] 33gJEFF-3.3 COV		Uncertainty [%] 56g ENDF/B-VIII.0 COV	
ESFR	k-eff	0.3%	1.04	± 2.5E-04	0.90	± 1.0E-04
	Coolant density	5%	25.69	± 1.2E-01	32.43	± 9.5E-02
	Doppler+300K	5%	4.25	± 5.4E-01	3.58	± 3.9E-01
	Control	3%	1.96	± 1.1E-02	1.56	± 7.1E-03
ASTRID	k-eff	0.3	0.97	± 2.0E-04	0.89	± 5.4E-05
	Coolant density	5%	15.78	± 5.2E-02	18.33	± 3.4E-02
ALFRED	k-eff	0.435%	0.88	± 1.6E-04	0.85	± 4.7E-05
	Coolant density	5%	6.82	± 2.7E-01	5.77	± 8.4E-02
	Doppler+300K	5%	6.91	± 6.2E-01	5.21	± 2.5E-01

# IRPhE database

- Data from 167 experimental series performed at 56 nuclear facilities in the 2020 edition

## International Handbook of Evaluated Reactor Physics Benchmark Experiments



# Our experience with IRPhEP

- **Identification of benchmark experiments** useful to assess ND libraries for large SFRs
  - Core multiplication factor (some benchmarks are additionally as criticality experiments in ICSBEP)
  - Reactivity effects: Sodium void worth, Control rod worth, Temperature effect
- **Benchmarking and ND Validation with UQ:** C/E results for analyses of biases and trends
- **Data Assimilation**

# Identification of experiments useful for SFR

- **Experiments with a high similarity** to ESFR sensitivity profiles

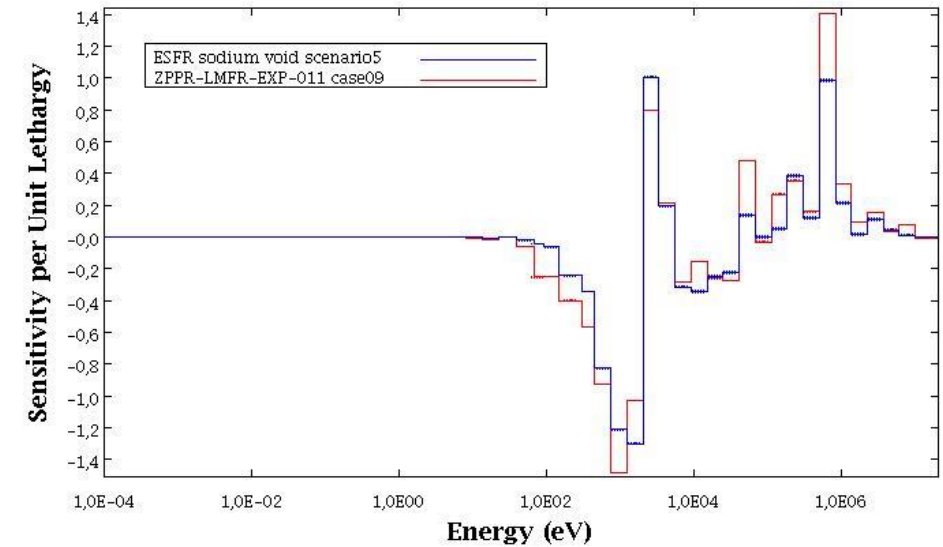
$$c_k = \frac{S_R^T M_\sigma S_E}{\sqrt{(S_R^T M_\sigma S_R)(S_E^T M_\sigma S_E)}}$$

$S_R$ : sensitivity vector for the targeted reactor (ESFR)

$S_E$ : sensitivity vector for the experiment

$$E = \frac{S_R^T S_E}{\sqrt{(S_R^T S_R)(S_E^T S_E)}}$$

- **Filter-based experiments**, imposing that detailed input for MCNP or KENO is provided along with the documentation (no simplified models considered for IRPhE-based V&V)



*Relative sensitivity coefficients of SVR to pu-239 (n.fission) for the ESFR design. For other SFR (i.e. ASTRID) similar sensitivities for k-eff but differences for SVR*

# Identification of experiments useful for SFR

- **Experiments with a high similarity** to ESFR sensitivity profiles

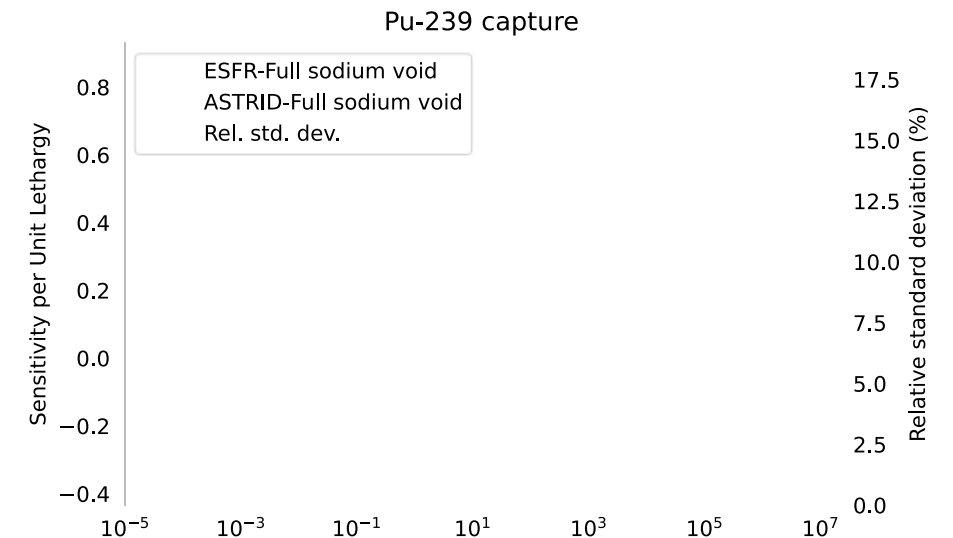
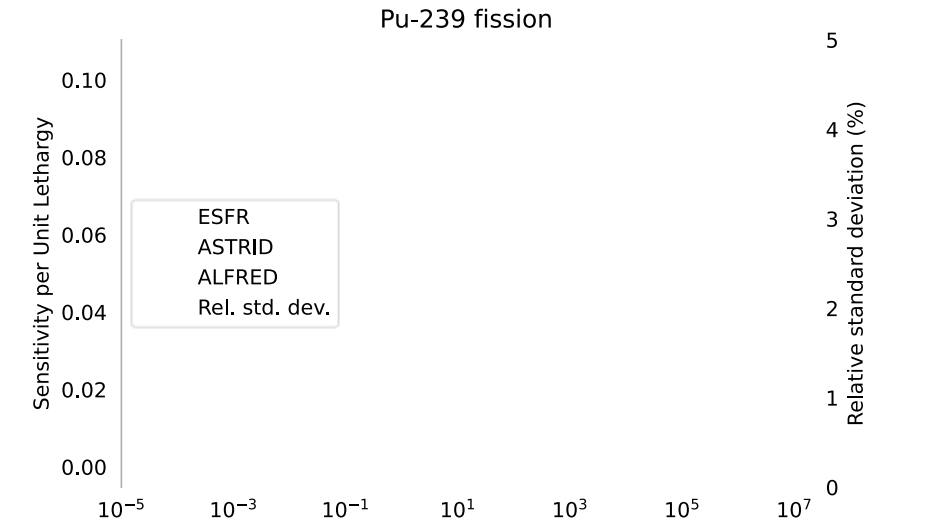
$$c_k = \frac{S_R^T M_\sigma S_E}{\sqrt{(S_R^T M_\sigma S_R)(S_E^T M_\sigma S_E)}}$$

$S_R$ : sensitivity vector for the targeted reactor (ESFR)

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- **Filter-based experiments**, imposing that detailed input for MCNP or KENO is provided along with the documentation (no simplified models considered for IRPhE-based V&V)



## SELECTION OF EXPERIMENTS USEFUL FOR K-EFF

Experiment	IRPhE identification	Additionally in ICSBEP	Description	Experimental value	Ck	E
BFS-97-1 Assembly	BFS1-FUND-EXP-001-001	MIX-MISC-MIXED-001	Critical assembly with heterogeneous compositions of plutonium, depleted-uranium dioxide, and polyethylene	1.001 ± 0.0029	0.88	
BFS-49-1 Assembly	BFS1-FUND-EXP-004-001	MIX-MISC-FAST-002-001	Critical experiments with heterogeneous compositions of plutonium, depleted-uranium dioxide, and polyethylene	1.0005 ± 0.0021	0.94	
BFS-61-1 Assembly	BFS1-LMFR-EXP-002-001	MIX-MET-FAST-006?	Experimental model of lead-cooled fast reactor with core of metal Pu, depleted uranium fuel and ≠ reflectors	1.0003 ± 0.0029		
FFTF initial isothermal measurements	FFTF-LMFR-RESR-001-001	-	Fast Flux Test Facility, a prototypic liquid metal fast breeder reactor, MOX-fuelled, sodium-cooled, Inconel-reflected core	0.9993 ± 0.0021	0.93	
SNEAK 7A	SNEAK-LMFR-EXP-001-001	MIX-MISC-FAST-002-001	Fast critical assemblies in the Karlsruhe fast critical facility, PuO <sub>2</sub> -UO <sub>2</sub> graphite core, reflected by metallic depleted U	1.001 ± 0.0035	0.93	
ZEBRA Assembly 22	ZEBRA-LMFR-EXP-001-001	-	ZEBRA Zero Power Critical Facility with plate form (22 and 24) and pin geometry form (23 and 25)	1.0022 ± 0.0008		
ZEBRA Assembly 23	ZEBRA-LMFR-EXP-001-002	-		1.0016 ± 0.0013		
ZPPR-10A Loading 7	ZPPR-LMFR-EXP-001-001	-	ZPPR-10A Experiment: A 650 MWe SFR MOX-fueled with 2 homogeneous Zones	1.0011 ± 0.0015		
ZPPR-9 Loading 13	ZPPR-LMFR-EXP-002-001	-	ZPPR-9 Experiment: A 650 MWe SFR MOX-fueled with clean core of 2 homogeneous zones	1.0008 ± 0.00154	0.79	

## SELECTION OF EXPERIMENTS USEFUL FOR K-EFF

Experiment	IRPhE identification	Additionally in ICSBEP	Description	Experimental value	Ck	E
ZPPR-13A Loading 24	ZPPR-LMFR-EXP-007-001	-	ZPPR-13A: A 650 MWe SFR, radial heterogeneous core with central blanket zone and two internal blanket rings	0.9996 ± 0.0015	0.883	
ZPPR-12 Loading 9	ZPPR-LMFR-EXP-010-001	-	ZPPR-12 had a clean, cylindrical, single-zone core. Reference critical configuration	1.0008 ± 0.0008	0.942	
ZPPR-2 Loading 90	ZPPR-LMFR-EXP-011-001	MIX-COMP-FAST-006	Cylindrical assembly with mixed (Pu,U)-Oxide fuel and sodium reflected by Du, sodium and steel	1.0005 ± 0.0007		
ZPR-3 Assembly 53 Loading 18	ZPR-FUND-EXP-006-001	MIX-MET-INTER-004	Cylindrical assembly of plutonium metal, depleted uranium and graphite with a thick depleted uranium reflector	0.9757 ± 0.0023	0.933	
ZPR-3 Assembly 54 Loading 11	ZPR-FUND-EXP-007-001	MIX-MET-INTER-003	Cylindrical assembly of plutonium metal, depleted uranium and graphite with a thick iron reflector	0.9638 ± 0.0027	0.929	
ZPR-9 Assembly 31 Loading 22	ZPR-FUND-EXP-014-001	MIX-COMP-FAST-005-001	Cylindrical assembly with mixed (Pu,U)-Carbide fuel and depleted uranium carbide blanket	0.9913 ± 0.0023		
ZPR-6/7 Loading 41	ZPR-LMFR-EXP-001-001	MIX-COMP-FAST-001	ZPR-6 Assembly 7 Experiments: Fast reactor core with MOX fuel and sodium with a thick depleted uranium reflector	1.0005 ± 0.0009	0.782	
ZPR-6/7 Loading 99	ZPR-LMFR-EXP-002-001	MIX-COMP-FAST-002	ZPR-6 Assembly 7 Experiments: Fast reactor core with MOX fuel and a central high Pu-240 zone	1.0008 ± 0.0009	0.785	

## SELECTION OF EXPERIMENTS USEFUL FOR SODIUM VOID WORTH

Experiment	IRPhE identification	Cases	Description	Experimental value	Ck	E
ZPPR-12	ZPPR-LMFR-EXP-010	Loading 26: Base	Base configuration for the void worth measurements for the plate-loaded ZPPR-12		-	
		Loading 30	Zones 1-3 voided			
		Loading 33	Zones 1-6 voided			
		Loading 37	Zones 1-9 voided (the entire core)			
ZPPR-2	ZPPR-LMFR-EXP-011	Loading 177 (ref0409)	Base configuration for the void worth measurements		-	
		Loading 184 (case 8)				
		Loading 185 (case 9)		195.42 ± 5.1 %	0.918	

### SELECTION OF EXPERIMENTS USEFUL FOR CONTROL ROD WORTH

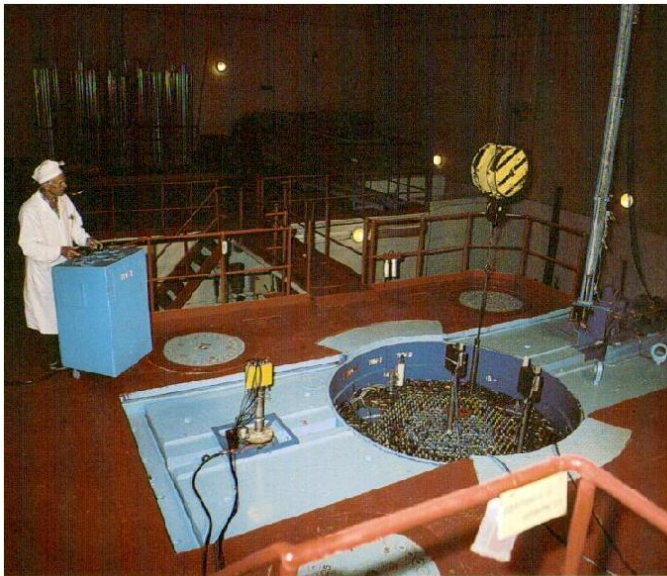
Experiment	IRPhE identification	Cases	Description	Experimental value	Ck	E
FFTF	FFTF-LMFR-RESR-001	ARI	Fully Subcritical ARI (All Rods In)	-	-	-
		Case 22	Primary bank withdrawn. Reference state: Fully Subcritical ARI			
		Case 23	Secondary bank withdrawn. Reference state: Fully Subcritical ARI			
		State1	Subcritical State 1 for shutdown margin	-	-	-
		Case 30	Rods dropped: all. Reference state: Subcritical State 1			
		State2	Subcritical State 2 for shutdown margin	-	-	-
		Case 31	Rods dropped: all. Reference state: Subcritical State 2			
		Case 32 (ARO)	All Rods Withdrawn. Reference state: critical core configuration			

### SELECTION OF EXPERIMENTS USEFUL FOR DOPPLER EFFECT

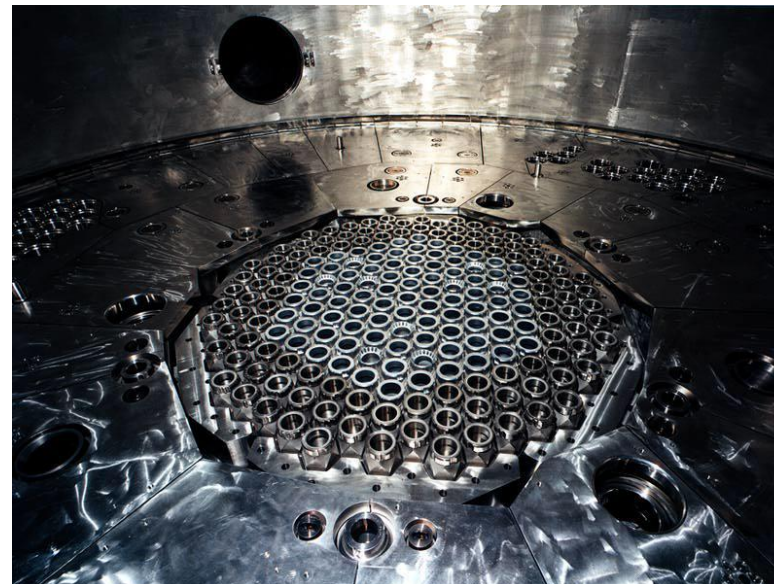
Experiment	Identification	Cases	Description	Experimental value	Ck	E
NOT in IRPhEP Selected in UAM-SFR	SEFOR	Core-I-E	South-West Experimental Fast Oxide Reactor, SFR with PuO <sub>2</sub> -UO <sub>2</sub>			
		Core-II-C				

**Summary:** identification of a set of benchmark experiments in IRPhEP useful to assess ND libraries for large SFR

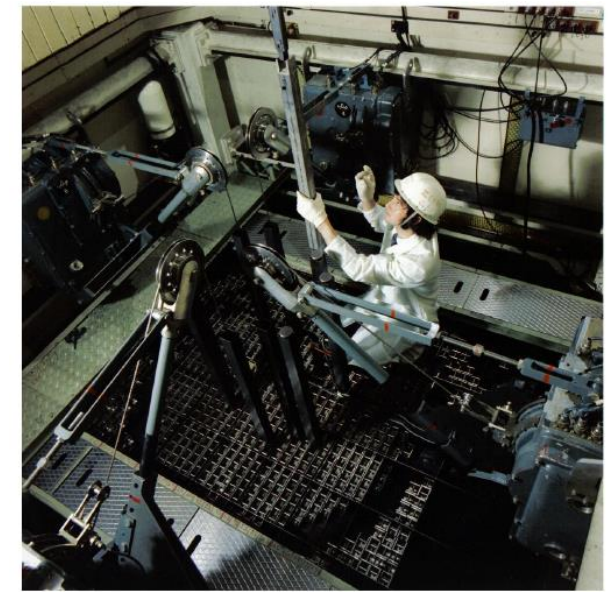
- 17 experiments for multiplication factors
- 10 experiments for reactivity effects



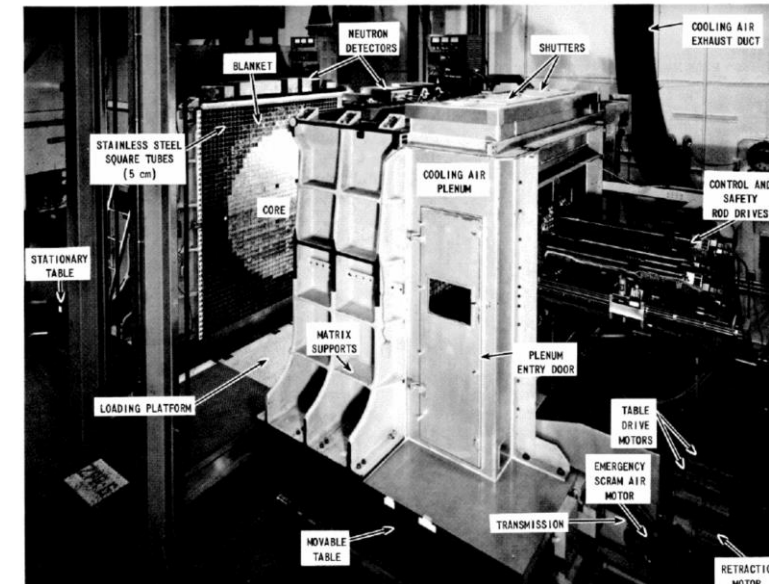
**BFS-1 Critical Facility** at Institute Physics and Power Engineering (IPPE), Obinsk, Russia



**Fast Flux Test Facility** at Handford site in Washington



**ZEBRA** (Zero Energy Breeder Reactor Assembly) Zero Power Critical Facility at UKAEA

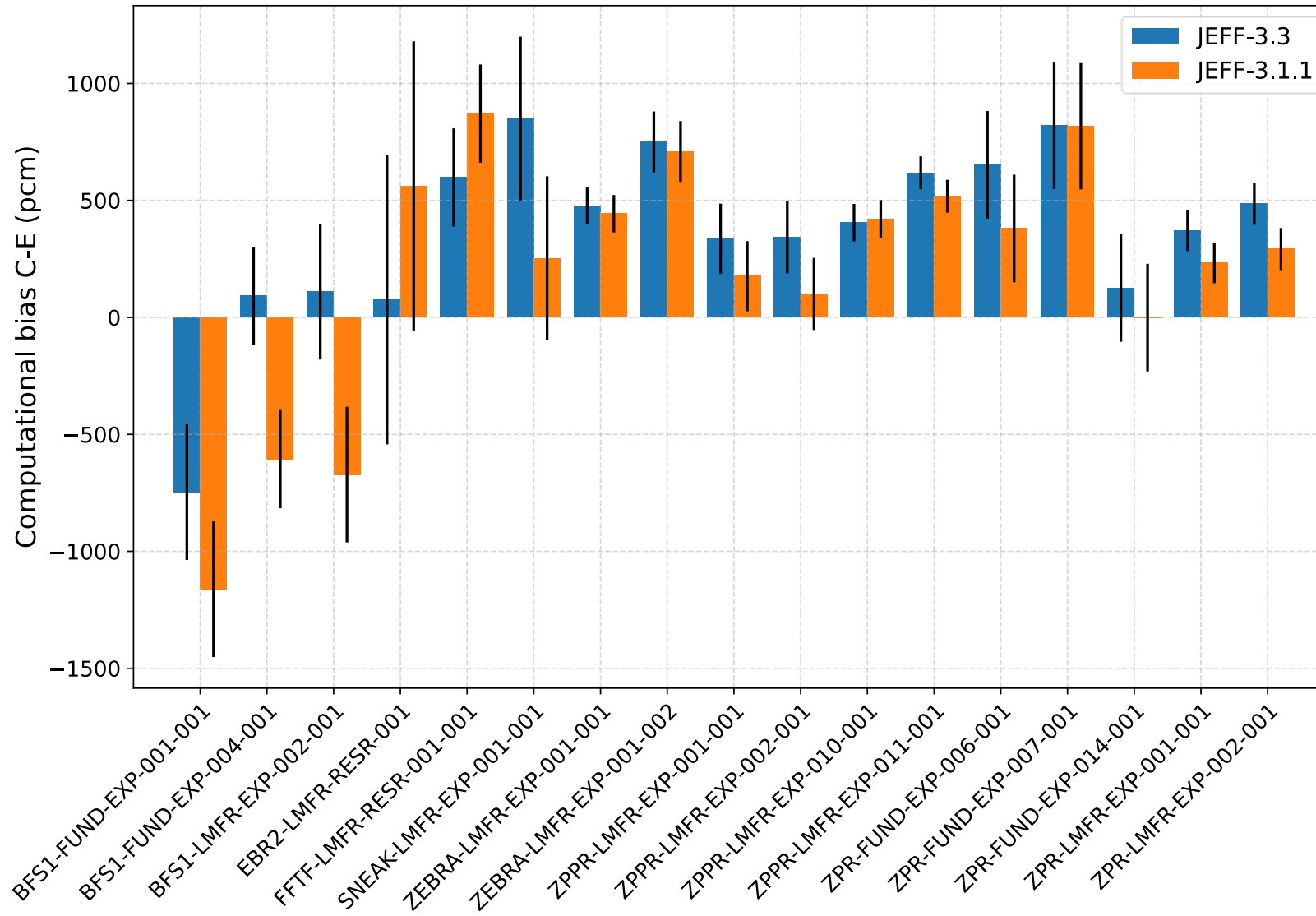


**ZPR-6** (Zero Power Reactor) Facility at Argonne National Laboratory

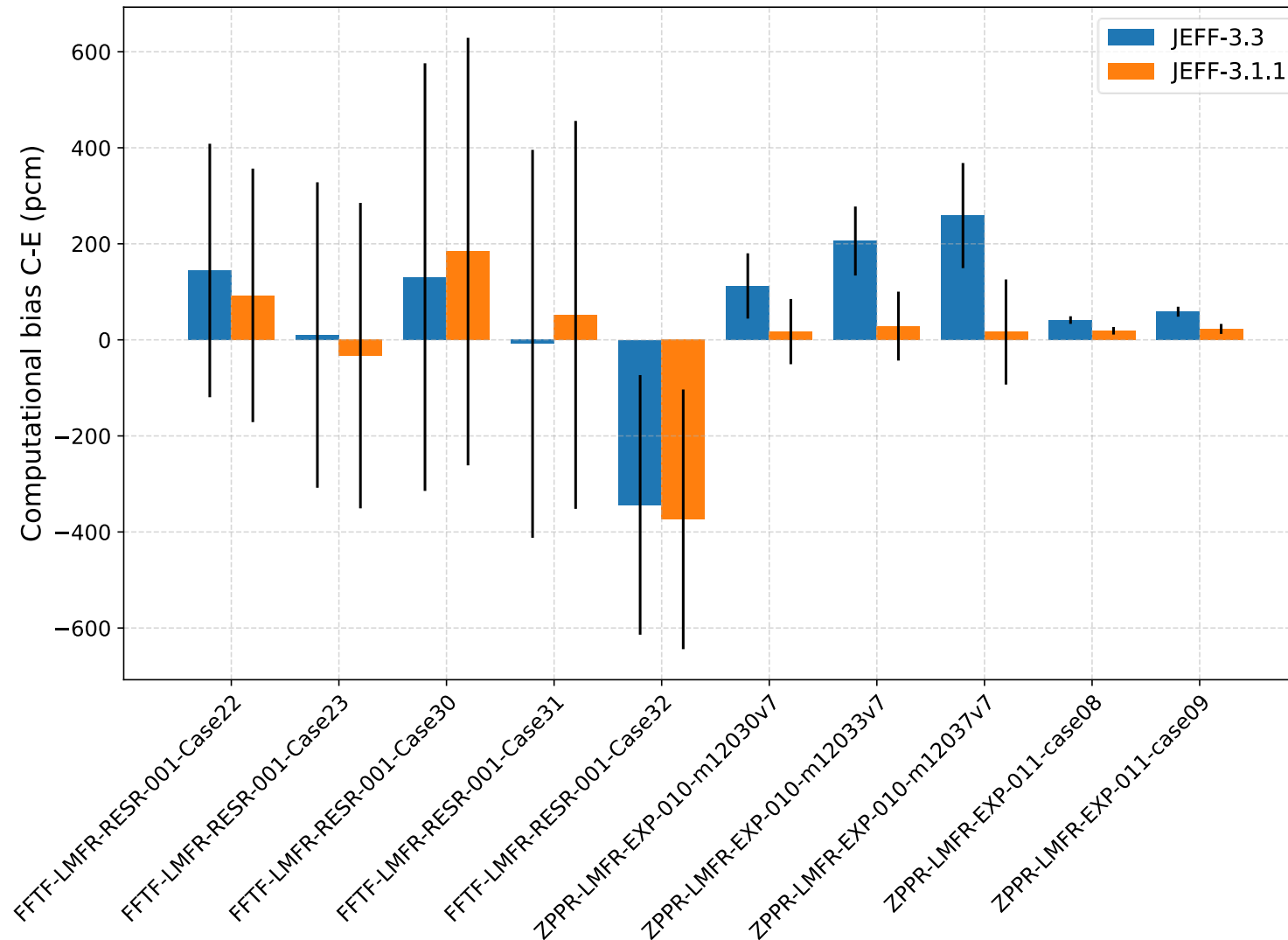
# Computational tools and data

- Criticality calculations with **MCNP6.2** with  $5 \cdot 10^8$  active neutron histories
  - Statistical uncertainties in k-eff  $\sim$  2-3 pcm, lower than benchmark uncertainties ( $> 70$  pcm in all cases)
  - Sensitivities computed with KSEN in 33g : available in .sdf format
- Nuclear data libraries from OECD/NEA:
  - **JEFF-3.3**: ACE files, NDEC-njoy 2016.42 at NEA on 2018-10-01
  - **JEFF-3.1.1**: from JEFF3.1.1 NJOY99.040\_up259, NEA\_Dic2008
- Uncertainty analysis and Data assimilation with SCALE6.3beta11
  - **JEFF-3.3 COV**: COVERX-formatted matrix processed with AMPX in 33g

# C/E results for k-eff



# C/E results for reactivity effects



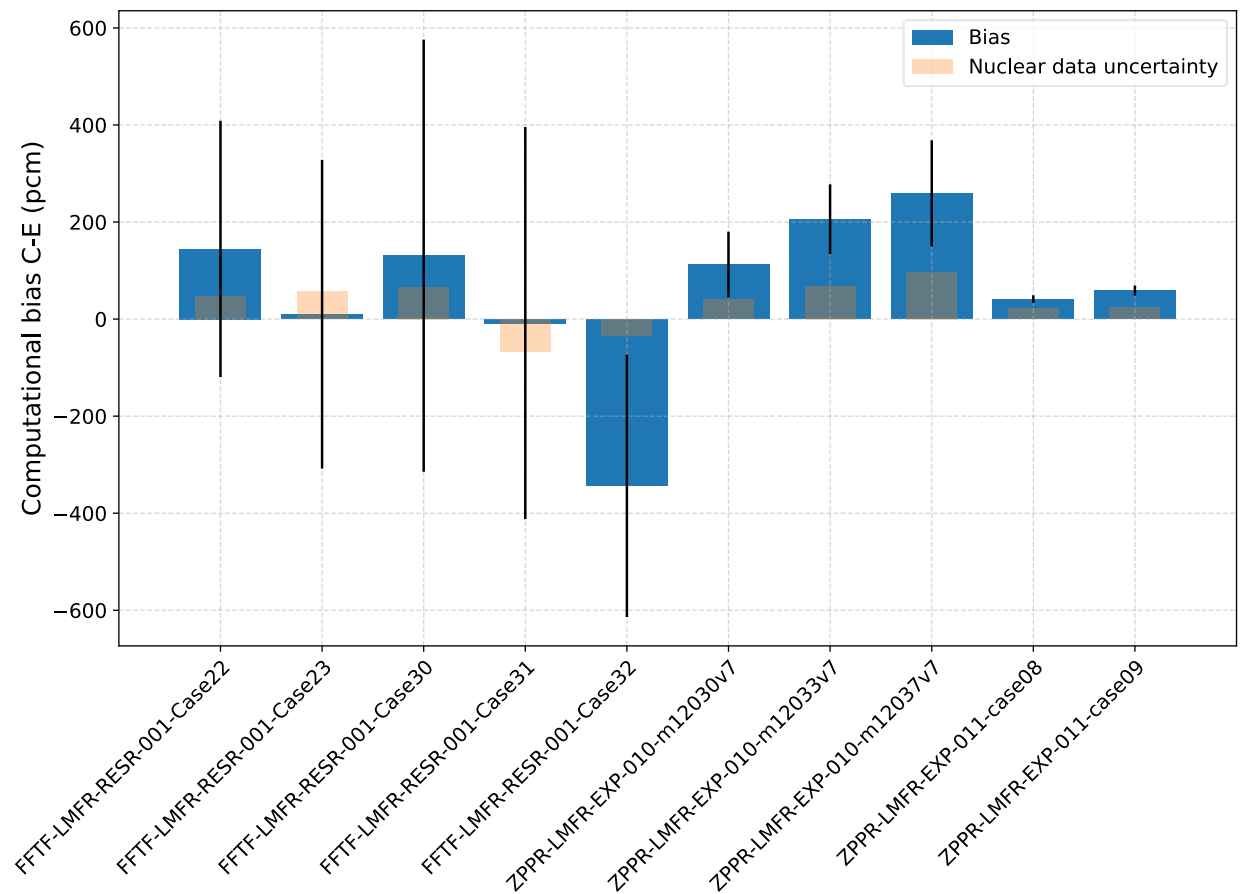
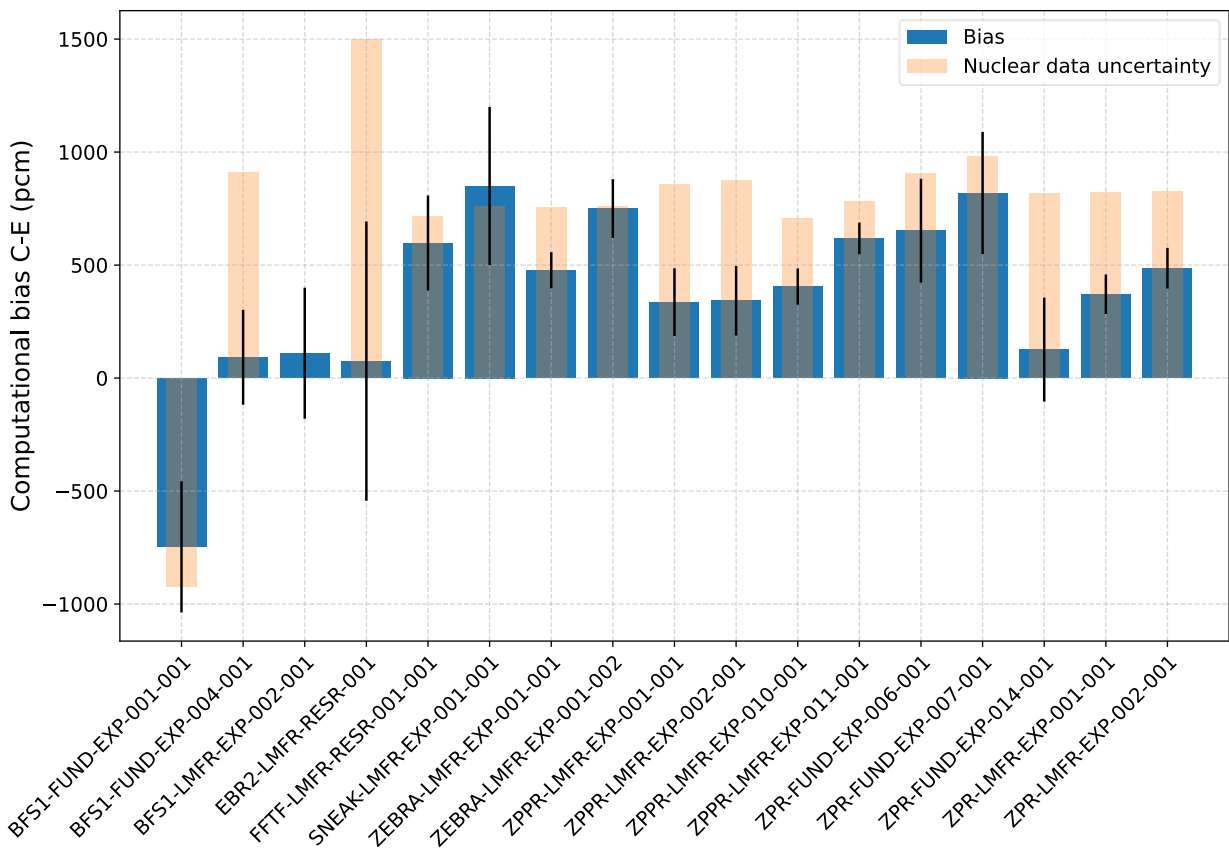
# ND Sensitivities

- Used to evaluate uncertainties in the output quantities
- Used to identify the origin of the biases between libraries through NDaST / NEA and Data Assimilation techniques
- Used to rank the isotope-reactions contributing the most to each experiment and guide the validation process for specific ND

	pu-239 fission	pu-239 nu-fission	pu-239 n,gamma	u-238 fission	u-238 nu-fission	u-238 fission	u-238 n,gamma	u-238 elastic	fe-56 elastic	na-23 elastic	o-16 elastic	b-10 n,alpha	b-11 elastic
FFTF-LMFR-RESR-001-Case22	-8,5E-01	-7,9E-01			-1,4E-01							4,4E-01	1,4E-01
FFTF-LMFR-RESR-001-Case23	-8,5E-01	-7,7E-01			-1,6E-01	-1,3E-01						4,3E-01	
FFTF-LMFR-RESR-001-Case30	8,5E-01	7,9E-01			1,4E-01							-4,5E-01	-1,3E-01
FFTF-LMFR-RESR-001-Case31	8,5E-01	7,8E-01			1,5E-01							-4,5E-01	-1,2E-01
FFTF-LMFR-RESR-001-Case32	-8,6E-01	-7,8E-01			-1,4E-01	-1,1E-01						4,4E-01	
ZPPR-LMFR-EXP-010-m12030v7			7,8E-01	6,8E-01	9,9E-01					-1,6E+00	1,0E+00		
ZPPR-LMFR-EXP-010-m12033v7			6,5E-01	5,8E-01	8,5E-01					-1,3E+00	6,1E-01		
ZPPR-LMFR-EXP-010-m12037v7	5,3E-01			4,9E-01	7,1E-01					-1,2E+00	5,0E-01		
ZPPR-LMFR-EXP-011-case08		-1,4E+00	8,5E-01				9,4E-01		1,1E+00		-1,2E+00		
ZPPR-LMFR-EXP-011-case09		-1,4E+00	8,4E-01				9,4E-01	7,7E-01		6,8E-01			



# ND Uncertainties compared to C/E

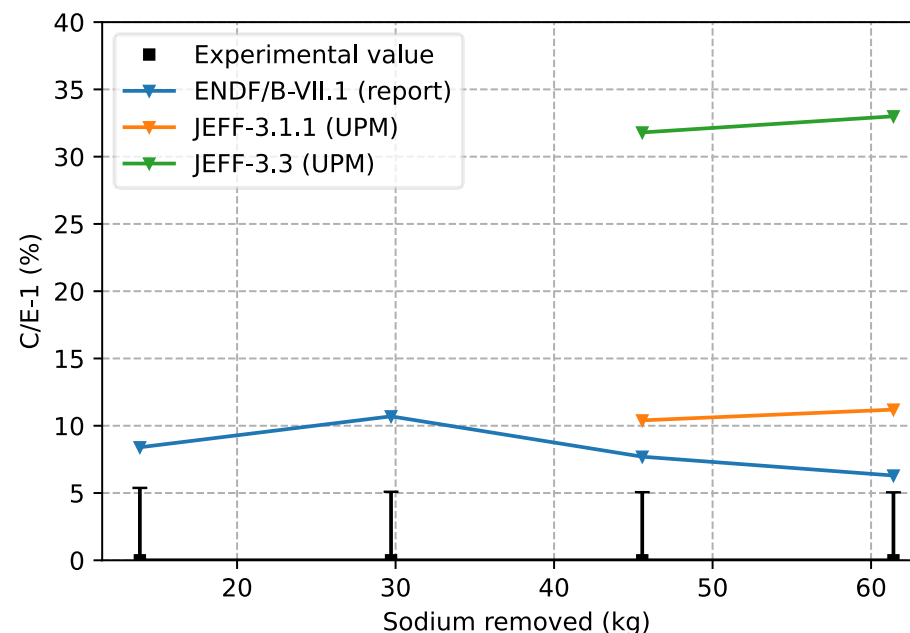
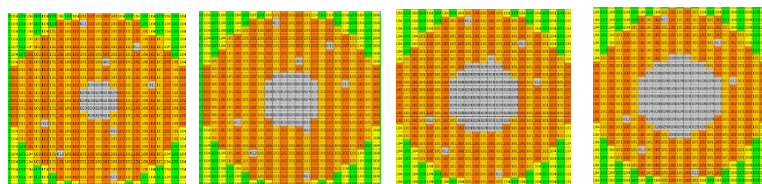


C/E deviations for JEFF3.3 compared to uncertainties due to JEFF3.3 covariance data

# Some trends investigated: ZPPR-2



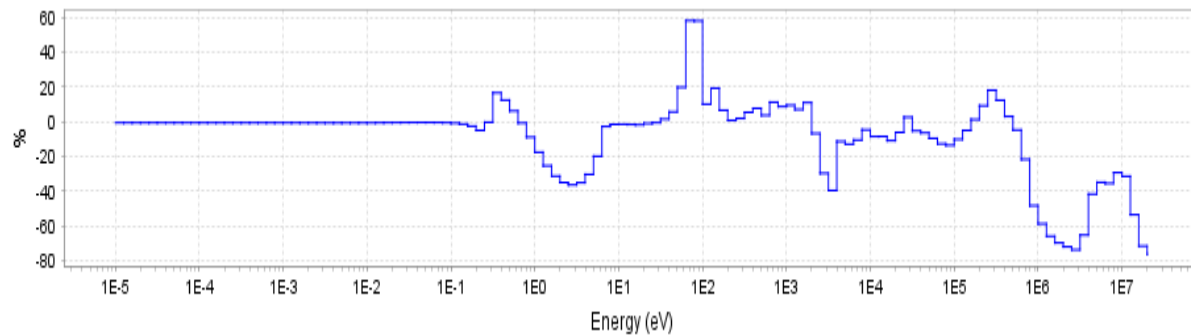
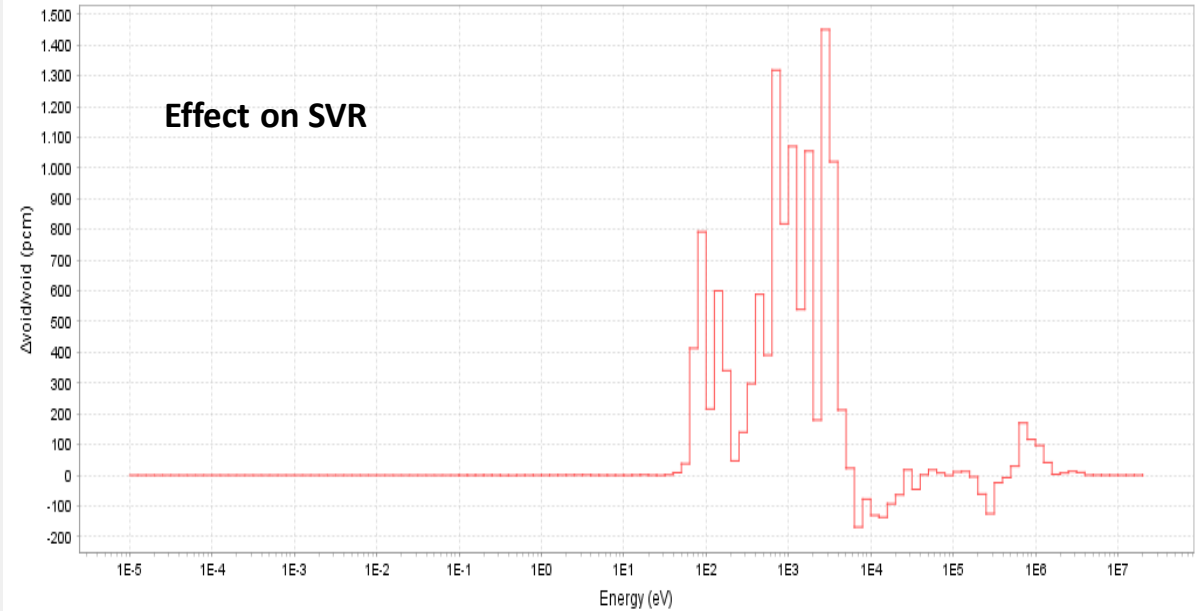
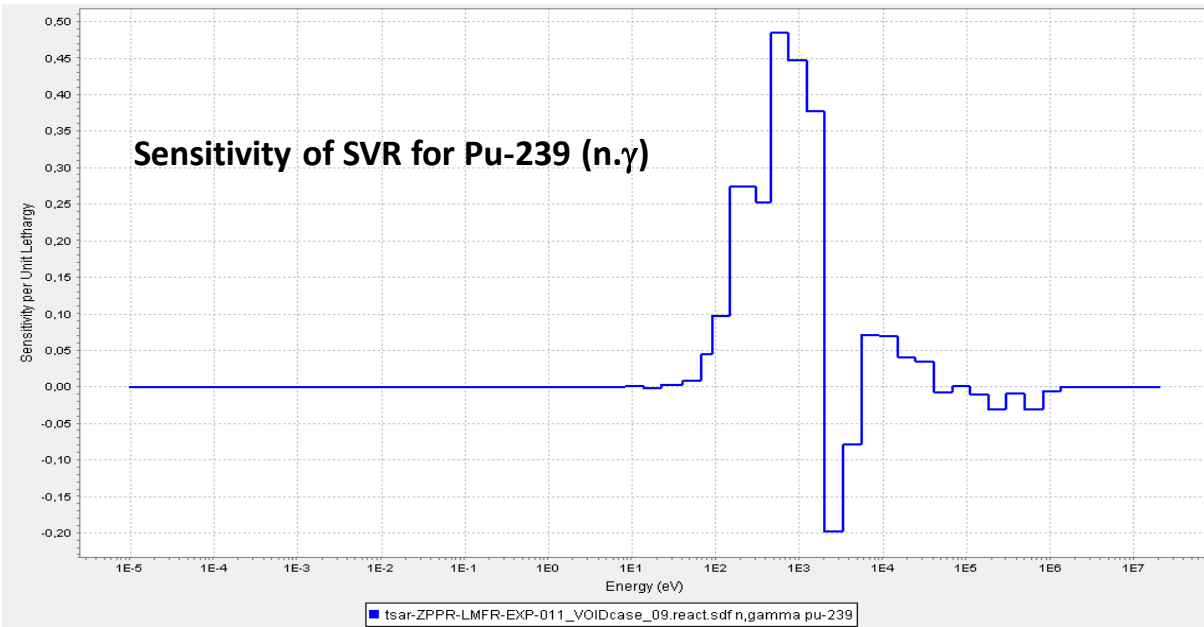
- Argonne National Laboratory Zero Power Plutonium Reactor ZPPR Assembly 2 (ZPPR-LMFR-EXP-011)
- Different core configurations. with different quantity of Na removed



worse agreement for JEFF-3.3 effect mainly due to Pu-239 (n,  $\gamma$ ) and fission ( $\sim 1$  keV)

Ref: N. García-Herranz. A. Jiménez-Carrascosa. O. Cabellos. F. Cháfer "UPM contribution to SANDA Task 5.2: Validation Studies using Existing Experiments". SANDA Project General Meeting. March 7-11. 2022

# Some trends investigated: ZPPR-2



**Pu-239 (n.g) ratio JEFF-3.3/JEFF-3.1.1**

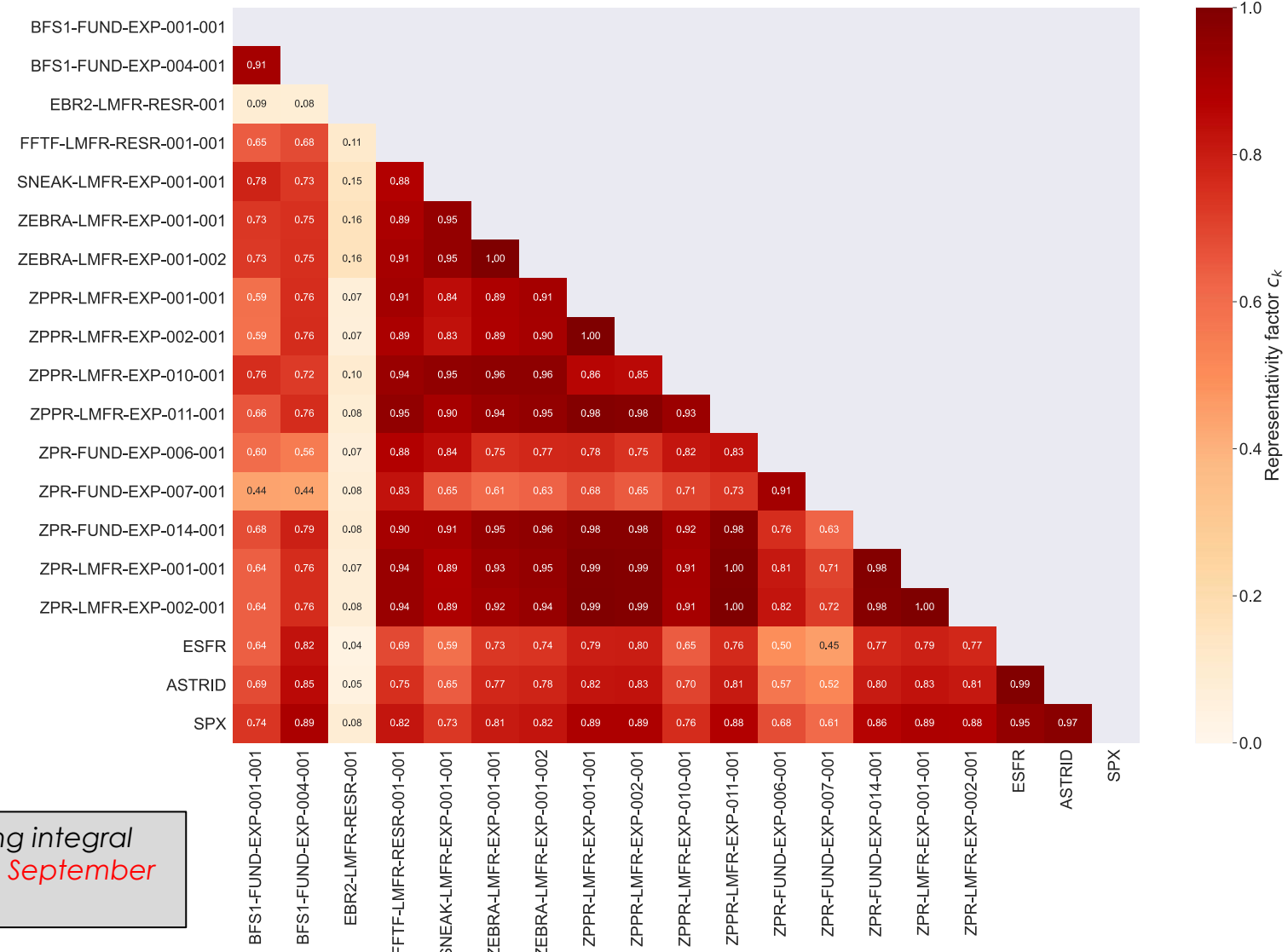
Use of NDaST/NEA to identify source of biases

Excellent benchmark to check performance of Pu-239 nuclear data



# Nuclear data assimilation

- Assimilation techniques can be used to transfer experimental information to ND library
- They may reveal potential ND biases
- Application of GLLS method using ICSBEP experiments\* led to a reduction of C/E biases for k-eff but not for reactivity effects : IRPhEP (ongoing)



\*Ref: A. Jiménez-Carrascosa et al., ND assimilation for SFR using integral experiments, Annual meeting of the Spanish Nuclear Society, September 28-30, 2022

# Summary

- Identification of a set of experiments in IRPhEP useful for ND assessment in SFR: **17 experiments for k-eff, 10 experiments for reactivity effects**
- **C/E results**: in general JEFF-3.3 provides higher deviations compared to JEFF-3.1.1 (relevant degradation for the SVR)
- **Sensitivities** to rank reactions, identify reactions responsible of biases and perform UQ due to nuclear data to analyze coverage
- **Data assimilation** to reveal potential ND biases: it is crucial to include different integral parameters

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

# Backup slides



# ND Sensitivities

	pu-239 nubar	pu-239 fission	pu-239 n,gamma	u-238 nubar	u-238 n,gamma	u-238 elastic	u-238 fission	u-235 elastic	u-235 nubar	u-235 fission	u-235 n,gamma	fe-56 elastic	na-23 elastic	h-1 elastic
BFS1-FUND-EXP-001-001	8,1E-01	5,8E-01		1,6E-01	-1,4E-01									
BFS1-FUND-EXP-004-001	8,4E-01	4,6E-01												1,8E-01
EBR1138BKAsBuilt									9,6E-01	5,5E-01	-9,1E-02	6,7E-02	5,4E-02	
FFTF-LMFR-RESR-001-001	8,5E-01	5,8E-01	-6,9E-02	8,1E-02	-1,2E-01									
SNEAK-LMFR-EXP-001-001	8,0E-01	5,5E-01		1,3E-01	-1,6E-01	1,0E-01								
ZEBRA-LMFR-EXP-001-001	7,6E-01	5,3E-01		1,2E-01	-1,6E-01	8,8E-02								
ZEBRA-LMFR-EXP-001-002	7,6E-01	5,3E-01		1,2E-01	-1,7E-01	8,7E-02								
ZPPR-LMFR-EXP-001-001	8,1E-01	5,7E-01		1,3E-01	-2,4E-01		8,2E-02							
ZPPR-LMFR-EXP-002-001	8,0E-01	5,7E-01		1,4E-01	-2,5E-01		8,6E-02							
ZPPR-LMFR-EXP-010-001	8,4E-01	5,8E-01		1,0E-01	-1,3E-01		6,5E-02							
ZPPR-LMFR-EXP-011-001	8,2E-01	5,7E-01		1,2E-01	-2,0E-01		7,4E-02							
ZPR-FUND-EXP-006-001	8,9E-01	5,7E-01	-1,2E-01		-1,5E-01			1,7E-01						
ZPR-FUND-EXP-007-001	9,3E-01	5,8E-01	-1,4E-01					2,0E-01				1,0E-01		
ZPR-FUND-EXP-014-001	7,9E-01	5,7E-01		1,6E-01	-2,1E-01		9,6E-02							
ZPR-LMFR-EXP-001-001	8,0E-01	5,6E-01		1,2E-01	-2,2E-01		7,6E-02							
ZPR-LMFR-EXP-002-001	8,2E-01	5,8E-01		1,2E-01	-2,3E-01		7,6E-02							