

# **GRS Results for the Burnup Pin-cell Benchmark Propagation of Cross-Section, Fission Yields and Decay Data Uncertainties**

**J.S. Martinez <sup>(1, 2)</sup> , W. Zwermann <sup>(1)</sup> ,  
L. Gallner <sup>(1)</sup> , F. Puente-Espel <sup>(1)</sup> and O. Cabellos <sup>(2)</sup>**

<sup>(1)</sup> Gesellschaft für Anlagen- und Reaktorsicherheit  
(GRS) mbH, Munich, Germany

<sup>(2)</sup> Department of Nuclear Engineering,  
Universidad Politécnica de Madrid, Spain

## Outline

### **1. Introduction**

**1.1 the XSUSA Methodology**

**1.2 Extension to Fission Yields and Decay Data**

### **2. Problem and Results**

**2.1 Description of the Burnup Pin-cell Benchmark**

**2.2 Impact on k-eff of Cross-Sections, Fission Yields and Decay Data Uncertainties**

**2.3 Impact on Isotopic Evolution**

### **3. Conclusions and future work**

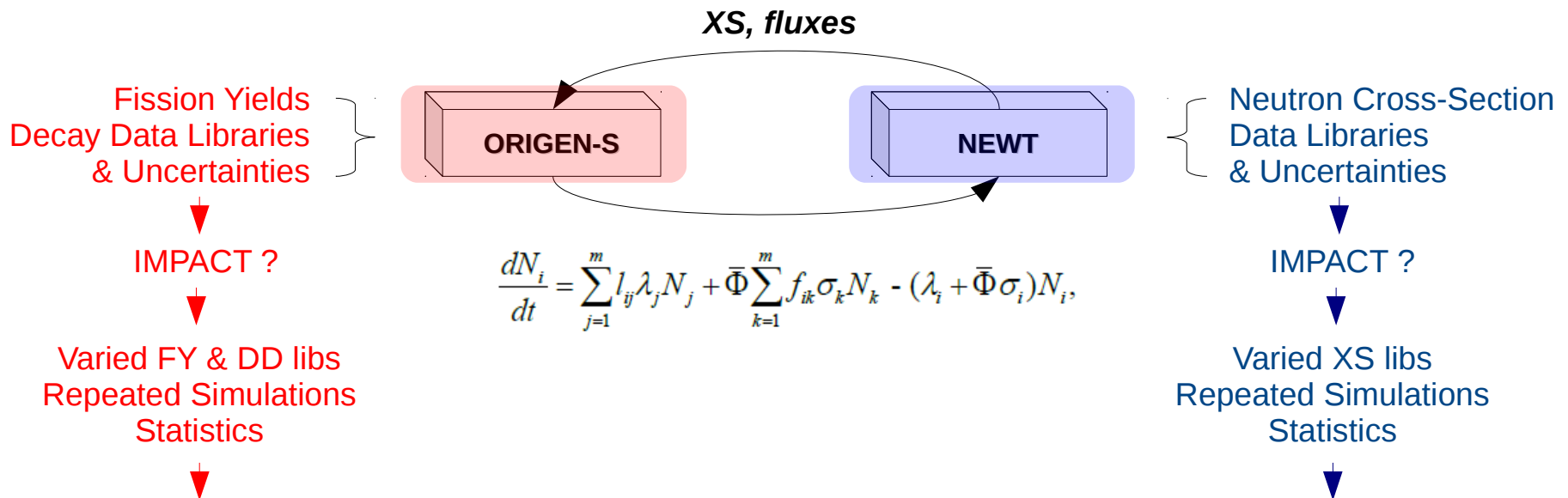
## 1. Introduction: the XSUSA Methodology

- Influence of Engineering Parameters and Cross-Section Uncertainties
- Many calculations (typically  $\gg 100$ ) are run for the same problem with varied input data
- Variations are generated randomly from the probability distributions of the input parameters and correlations between them
- Output quantities are statistically analyzed, uncertainty ranges and sensitivities are determined
- Applications:
  - Critical experiments.  
Transport calculations: multiplication factors, fission rate distributions
  - Full core calculations.  
MC and nodal diffusion: multiplication factors, power distributions  
Coupled nodal diffusion + thermo-hydraulics.
  - Fuel assembly depletion calculations.  
Multiplication factors, cross-sections, fission rates, nuclide inventories...
- XSUSA: Uncertainties through the generation of varied inputs and Cross-Sections (XS) and repeated simulation. **Fission Yields (FY) and Decay Data (DD) uncertainties not propagated**

**Regarding depletion calculations, XSUSA has been dealing with cross-section uncertainties BUT missing the contribution coming from the temporal evolution of the nuclide inventory**

- Accurate Burnup Simulation: Coupling between DEPLETION and TRANSPORT calculations

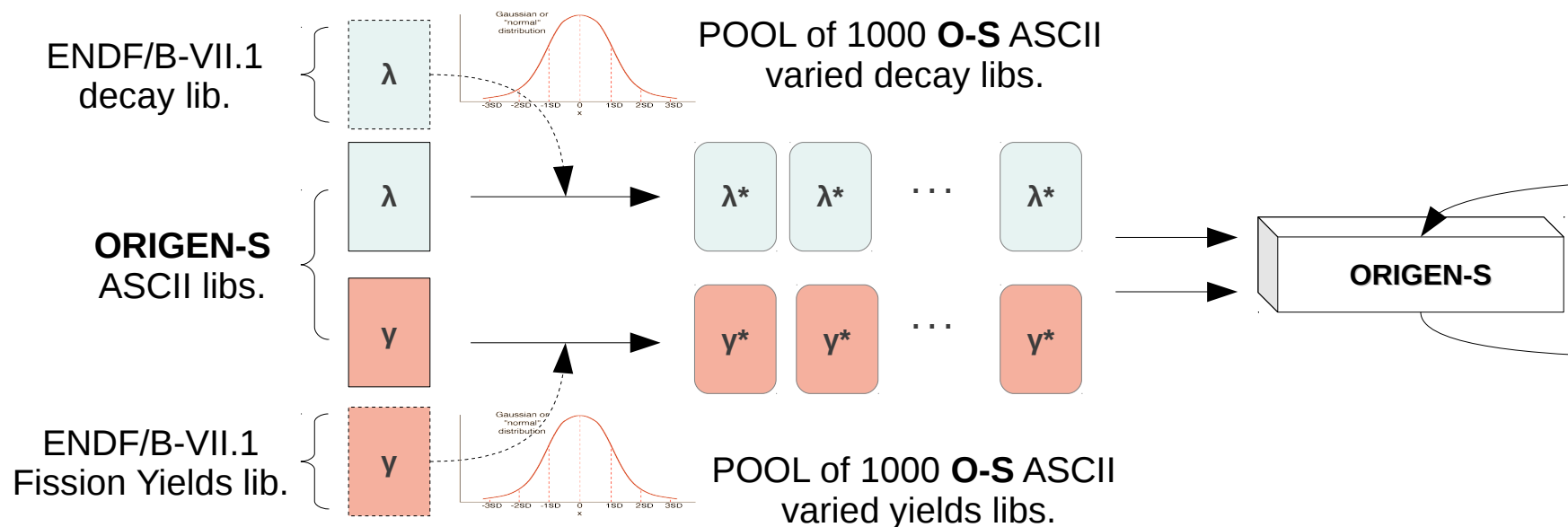
Isotopic Content Changes → Reaction Rates Changes



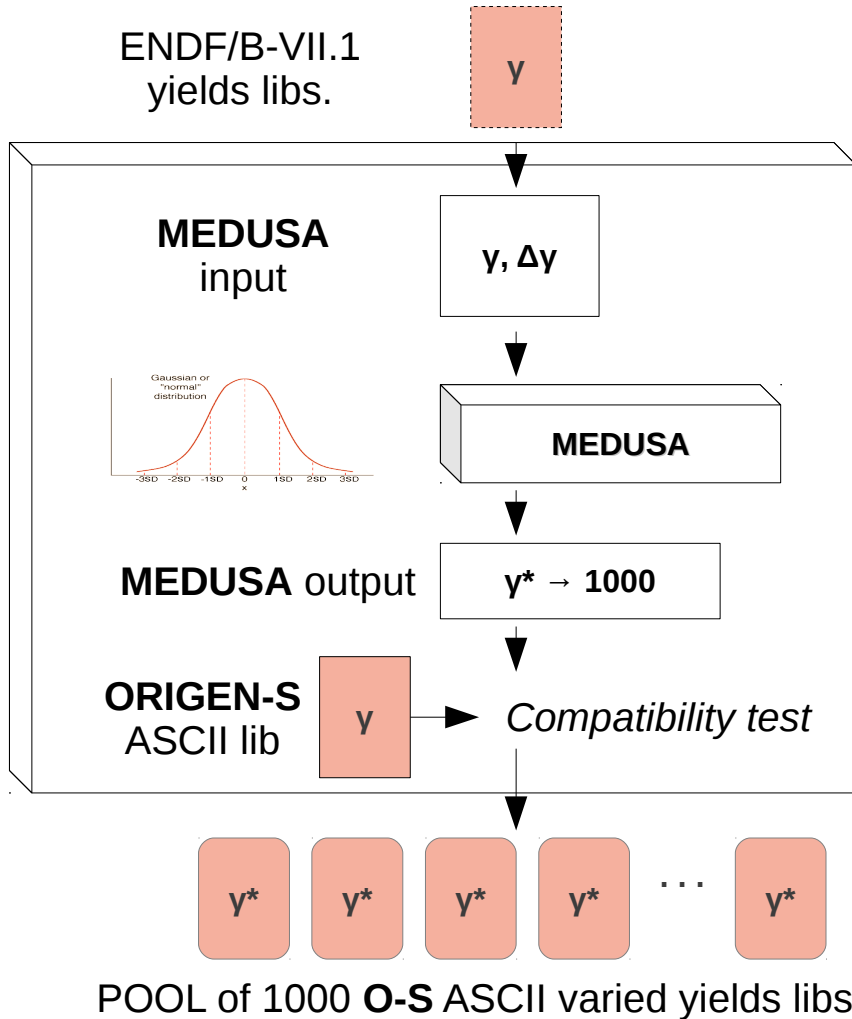
**Which is the impact on nuclear calculations of uncertainties coming from decay data, fission yields and cross-sections when considered independently and altogether ?**

# 1. Introduction: Extension to Fission Yields and Decay Data

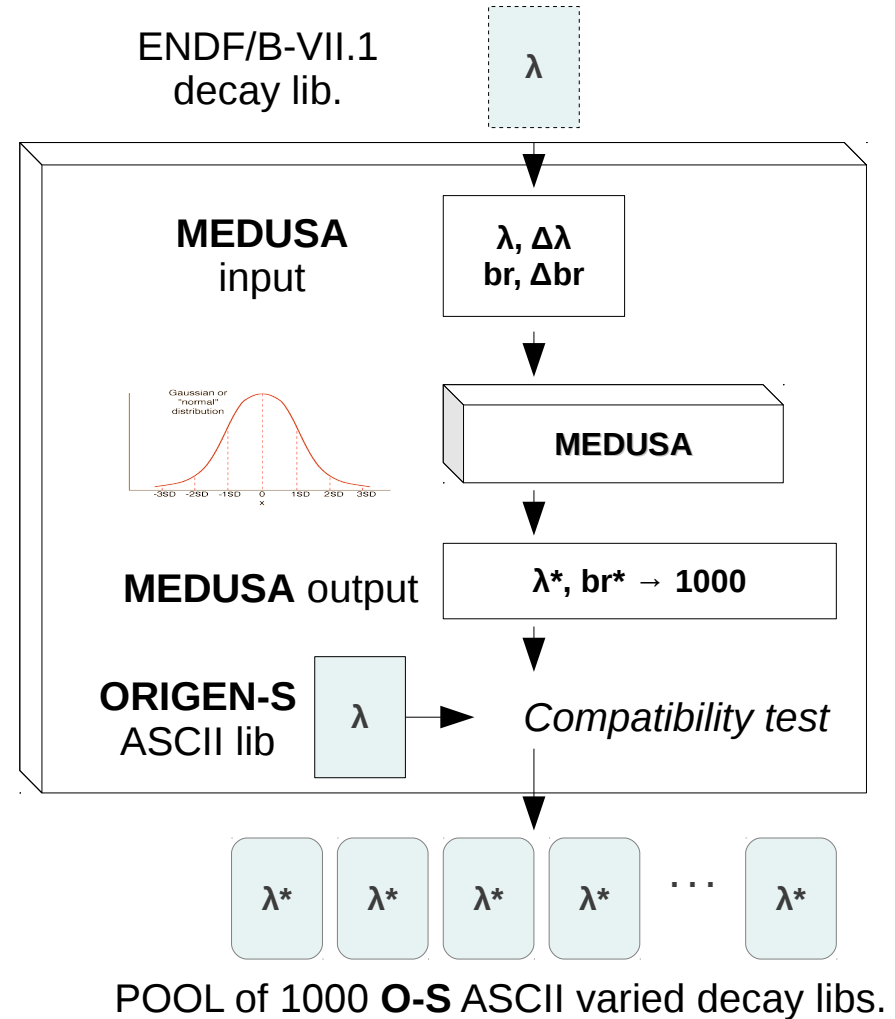
- XSUSA is updated to propagate uncertainties in Fission Yields and Decay Data
- XSUSA package includes two codes that generate pools of varied FY and DD libraries **beforehand**
- **We vary** the ORIGEN-S FY and DD libraries (**ASCII files**) **respecting the information they contain** (no additions, no replacements) according to the corresponding **uncertainties found in ENDF/B-VII.1** through a **gaussian sampling (MEDUSA)** around the **nominal values in ORIGEN-S libraries**



### YiSaB: XSUSA Yields Sampling Branch



### DeSaB: XSUSA Decay Sampling Branch



## 2. Problem and Results: Description of the Burnup Pin-cell Benchmark

### - The UAM-6 Burnup Pincell Benchmark (\*)

Unit cell pitch (mm)	14.427
Fuel pellet diameter (mm)	9.391
Fuel pellet material	UO <sub>2</sub>
Fuel density (g/cm <sup>3</sup> )	10.283
Fuel enrichment (w/o)	4.85
Cladding outside diameter (mm)	10.928
Cladding thickness (mm)	0.673
Cladding material	Zircaloy-4
Cladding density (g/cm <sup>3</sup> )	6.55
Gap material	He
Moderator material	H <sub>2</sub> O
Fuel temperature (K)	900.0
Cladding Temperature (K)	600.0
Moderator (coolant) temperature (K)	562.0
Moderator (coolant) density (g/cm <sup>3</sup> )	0.7484
Reactor Power (MWt)	2772.0
Total number of fuel assemblies	177
Number of fuel rods per fuel assembly	208
Active core length (mm)	3571.20

### Irradiation Characteristics

- simple pincell 4.85 % enrichment
- burnt at a constant power of **33.58 MW/MTU**
- during **1825 days** to a burnup of **61.28 GWd/MTU**
- total **decay time: 300 years**

### Data requested (at different time-steps)

- k-inf uncertainties
- Main nuclide reactions contributions + contribution of chi, nu-bar and others
- Reaction rates and uncertainties for major isotopes
  - capture for U<sub>235,238</sub> and Pu<sub>239,240,241</sub>
  - fission for U<sub>235,238</sub> and Pu<sub>239,240,241</sub>
  - two-group macroscopic cross sections and uncertainties for the homogenized pin-cell absorption, fission, nu-fission and diffusion
- Nuclide concentrations (15 Acts + 36 FPs)

\* BENCHMARK FOR UNCERTAINTY ANALYSIS IN MODELING (UAM) FOR DESIGN, OPERATION AND SAFETY ANALYSIS OF LWRs, Addition to V.I: Specification and Support Data for the Neutronics Cases (Phase I) "PWR Burnup Pin-Cell Benchmark" O. Cabellos and K.Ivanov

## Objectives

- Application of the extended XSUSA methodology to a simple test as a proof of principle
- Assessment of the impact on k-eff and the isotopic evolution of the independent and joint propagation of the different nuclear data uncertainties: XS, FY and DD

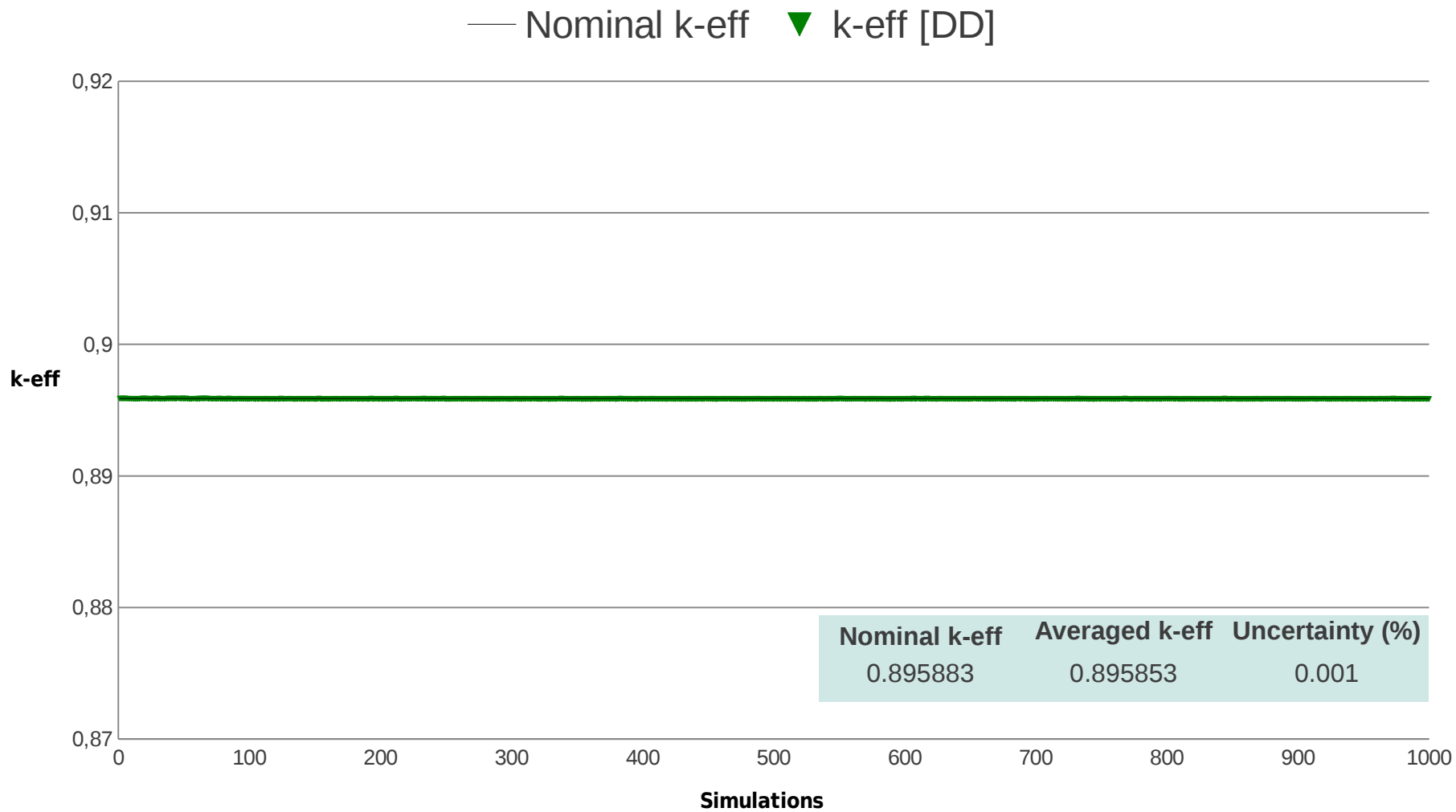
## Simulations performed

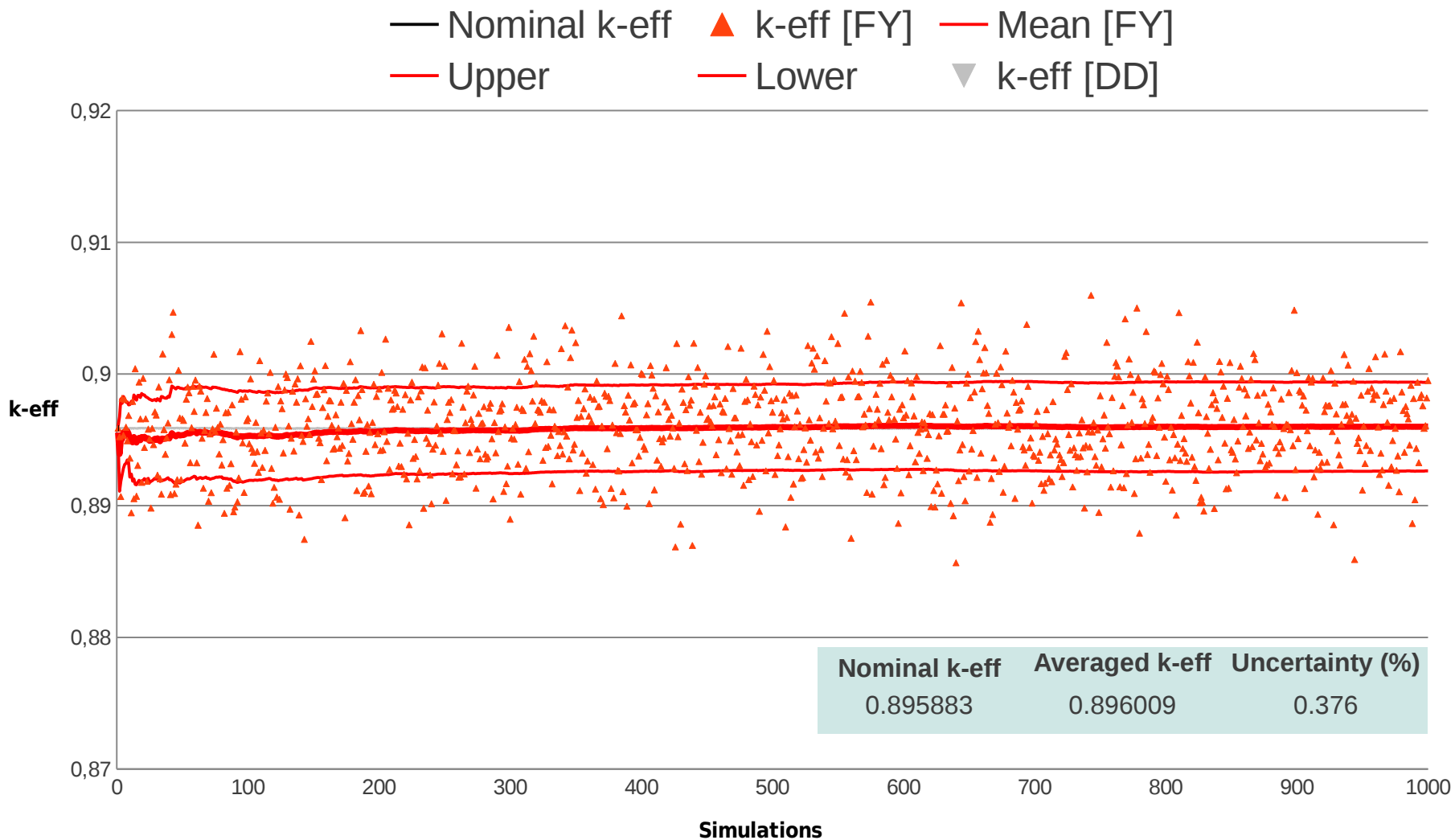
- Generation of 1000 of varied Fission Yields libraries and 1000 of varied Decay Data libraries
- Nominal calculation based on the original unchanged libraries
- Impact of DD → 1000 Burnup Calculations
- FY → "
- XS → "
- XS + FY + DD → "

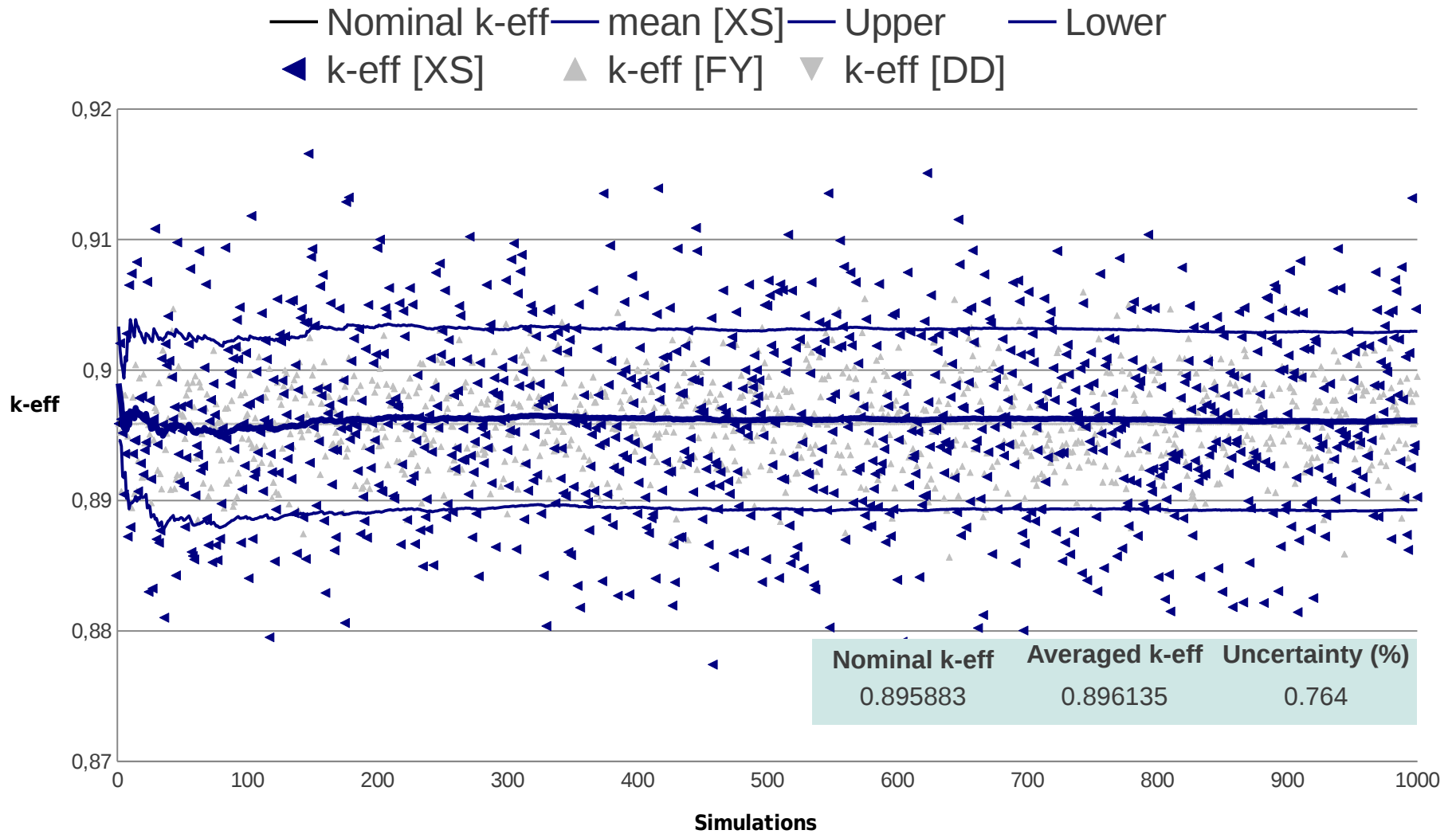
## Data Analyzed

- k-eff at EOB. Total Uncertainty and contribution from the different uncertainty sources
- Nuclide concentrations, uncertainties and contributions
- Comparison to the the results provided by other institutions



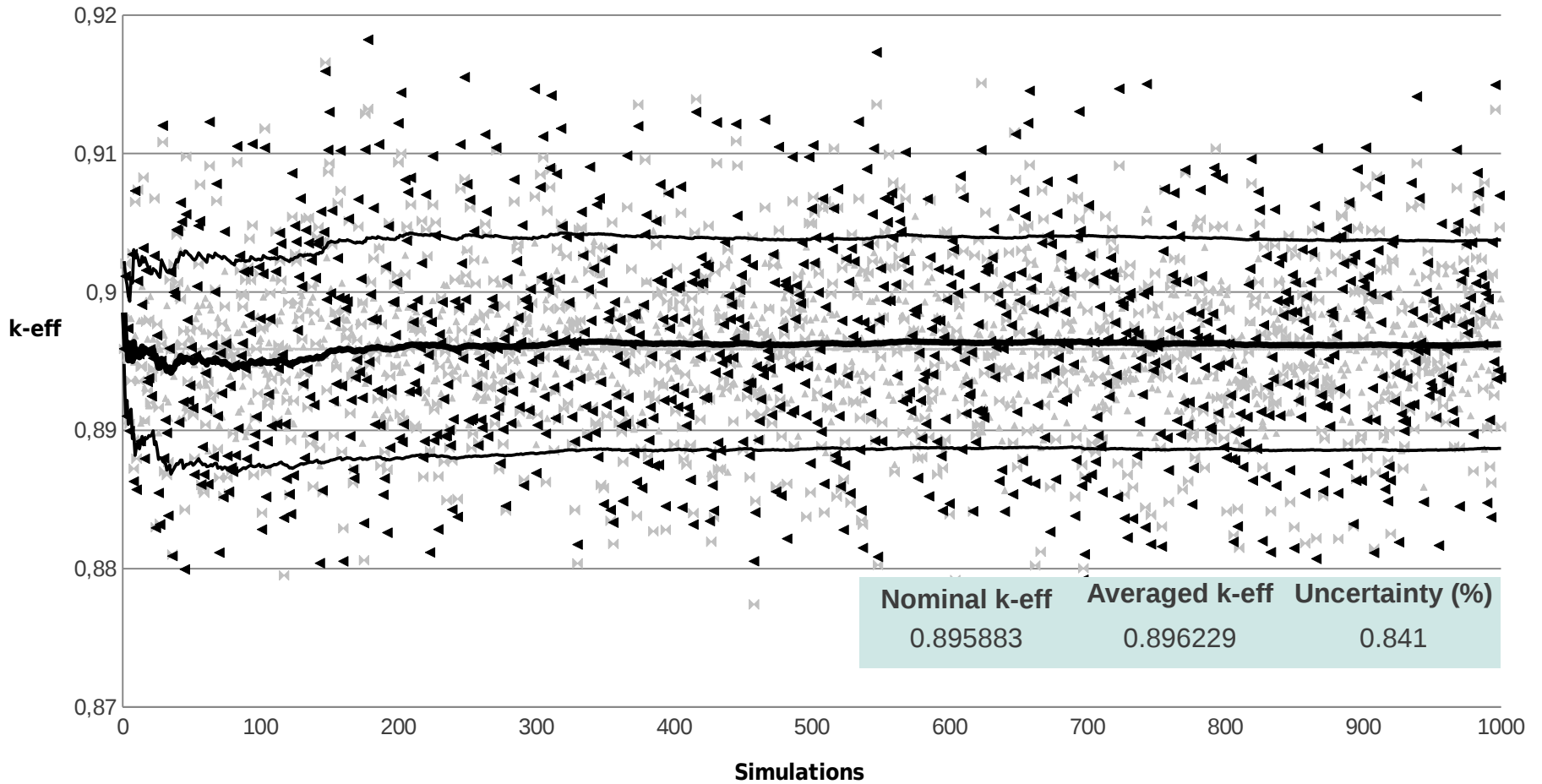


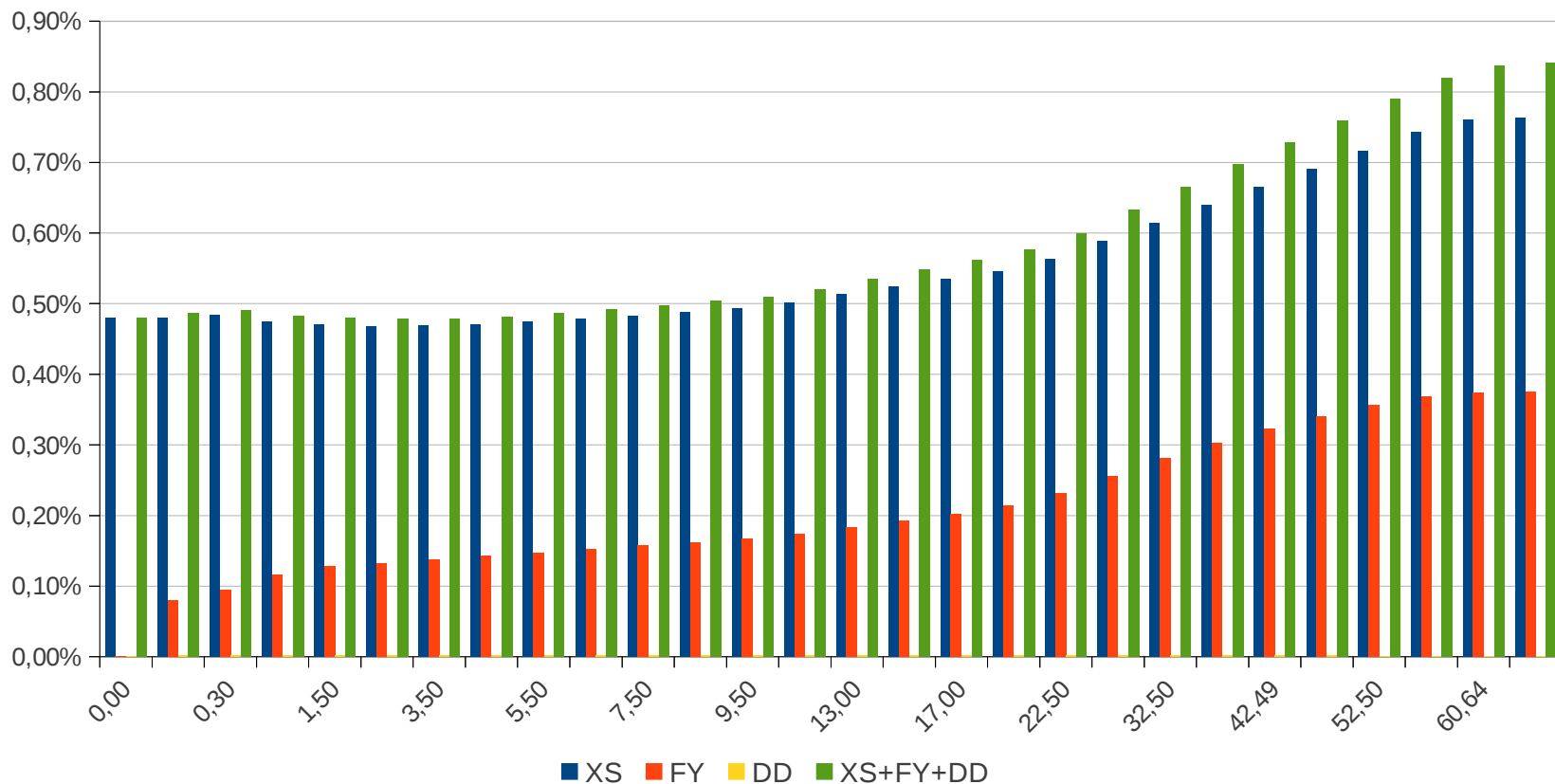






— Nominal k-eff    — mean [XS+FY+DD]    — Upper    — Lower  
◀ k-eff [XS+FY+DD]    × k-eff [XS]    ▲ k-eff [FY]    ▼ k-eff [DD]





**K-eff uncertainty finds its major contributor in XS > FY > DD (negligible) all over the irradiation**



Col.	Parm.	Var.	0 GWd/MTU	10 GWd/MTU	20 GWd/MTU	30 GWd/MTU	40 GWd/MTU	50 GWd/MTU	60 GWd/MTU	shutdown
UPM	Nom		1,4045	1,2461	1,1581	1,0837	1,0167	0,9560	0,9030	
	Uncert	Xs.	0.49%	0.51%	0.57%	0.63%	0.68%	0.74%	0.79%	
GRS	Nom		1,4029	1,2474	1,1623	1,0913	1,0270	0,9688	0,9169	0,9102
	Uncert	Xs	0,48%	0,49%	0,55%	0,60%	0,65%	0,70%	0,75%	0,75%
		FY	0,0%	0,17%	0,21%	0,28%	0,32%	0,36%	0,37%	0,38%
		Tot.	0,48%	0,51%	0,58%	0,67%	0,73%	0,79%	0,84%	0,84%
NRG	Nom		1,41	1,25	1,16	1,08	1,02	0,955	0,901	
	Uncert	U-235	0,50%	0,44%	0,39%	0,35%	0,32%	0,28%	0,24%	
		U-238	0,46%	0,48%	0,45%	0,40%	0,35%	0,33%	0,36%	
		Pu-239	0,05%	0,15%	0,26%	0,33%	0,39%	0,44%	0,47%	
		L FPs	0,05%	0,37%	0,36%	0,32%	0,23%	0,29%	0,28%	
		FY	0,05%	0,18%	0,19%	0,21%	0,21%	0,19%	0,17%	
		Tot.	0,68%	0,79%	0,78%	0,76%	0,76%	0,76%	0,79%	

		0 GWd/MTU		10 GWd/MTU			30 GWd/MTU			60 GWd/MTU				
		mean	mean	rel.	std. dev.	mean	rel.	std. dev.	mean	rel.	std. dev.			
				$\Delta$ XS	$\Delta$ DD	$\Delta$ FYs	$\Delta$ XS	$\Delta$ DD	$\Delta$ FYs	$\Delta$ XS	$\Delta$ DD	$\Delta$ FYs		
U-234	UPM	1.17E-05	1.03E-05	1.0	0.0	-	7.94E-06	1.9	0.0	-	5.04E-06	3.1	0.0	-
	NRG	1.17E-05	1.03E-05	0.1			7.92E-06	0.4			4.97E-06	0.9		
	GRS	1.13E-03	8.72E-04	0.8	0.0	0.02	4.98E-04	2.6	0.0	0.09	1.74E-04	5.7	0.0	0.30
U-235	UPM	1.13E-03	8.71E-04	0.2	0.0	-	4.97E-04	0.3	0.0	-	1.74E-04	0.6	0.0	-
	NRG	1.13E-03	8.75E-04	0.2			5.02E-04	0.7			1.75E-04	2.8		
	GRS	0.00E+00	4.87E-05	0.1	0.0	0.01	1.15E-04	0.5	0.0	0.06	1.58E-04	1.9	0.0	0.35
U-238	UPM	2.18E-02	2.17E-02	0.0	0.0	-	2.14E-02	0.1	0.0	-	2.08E-02	0.1	0.0	-
	NRG	2.18E-02	2.17E-02	0.0			2.14E-02	0.0			2.08E-02	0.0		
	GRS	0.00E+00	4.87E-05	0.01	0.0	0.0	1.15E-04	0.02	0.0	0.06	1.58E-04	0.04	0.0	0.35
Pu-238	UPM	0.00E+00	1.24E-07	2.3	0.0	-	2.08E-06	1.4	0.0	-	1.07E-05	0.9	0.0	-
	NRG	0.00E+00	1.22E-07	12.1			2.15E-06	5.0			1.14E-05	2.7		
	GRS	0.00E+00	8.07E-05	7.6	0.0	0.2	1.45E-04	4.4	0.0	0.24	1.57E-04	0.04	0.0	0.32
Pu-239	UPM	0.00E+00	8.08E-05	1.2	0.0	-	1.46E-04	1.1	0.0	-	1.60E-04	1.3	0.0	-
	NRG	0.00E+00	7.78E-05	1.8			1.40E-04	2.3			1.53E-04	3.2		
	GRS	0.00E+00	9.36E-06	1.2	0.0	0.1	4.00E-05	1.5	0.0	0.2	7.53E-05	2.0	0.0	0.46
Pu-240	UPM	0.00E+00	9.36E-06	3.1	0.0	-	4.01E-05	2.1	0.0	-	7.59E-05	1.9	0.0	-
	NRG	0.00E+00	9.09E-06	1.9			3.89E-05	2.0			7.39E-05	2.4		
	GRS	0.00E+00	3.55E-06	1.6	0.0	0.07	2.47E-05	1.9	0.0	0.11	4.67E-05	2.2	0.0	0.27
Pu-241	UPM	0.00E+00	3.55E-06	2.9	0.0	-	2.46E-05	1.7	0.0	-	4.68E-05	1.5	0.0	-
	NRG	0.00E+00	3.42E-06	2.0			2.42E-05	1.5			4.59E-05	2.2		
	GRS	0.00E+00	1.98E-07	1.6	0.0	0.16	4.96E-06	1.4	0.0	0.16	2.33E-05	1.8	0.0	0.32
Pu-242	UPM	0.00E+00	1.98E-07	3.7	0.0	-	4.95E-06	1.9	0.0	-	2.31E-05	1.4	0.0	-
	NRG	0.00E+00	1.92E-07	3.0			4.98E-06	1.9			2.40E-05	1.4		
	GRS	0.00E+00	1.98E-07	2.0	0.0	0.14	4.96E-06	2.3	0.0	0.10	2.33E-05	3.6	0.0	0.21

		0 GWd/MTU		10 GWd/MTU			30 GWd/MTU			60 GWd/MTU				
		mean	mean	rel. std. dev.	mean	rel. std. dev.	mean	rel. std. dev.	mean	rel. std. dev.				
				$\Delta XS$	$\Delta DD$	$\Delta FYs$								
Gd-155	UPM	0.00E+00	5.06E-10	12.4	0.2	5.1	2.23E-09	15.2	0.2	2.4	5.80E-09	15.4	0.2	1.1
	NRG	0.00E+00	5.06E-10	27.0			2.30E-09	22.4			6.02E-09	22.8		
	GRS	0.00E+00	1.56E-07	4.9	0.27	15	1.34E-06	6.0	0.24	9.8	7.63E-06	5.3	0.20	8.8
Nd-143	UPM	0.00E+00	1.23E-05	0.6	0.0	2.6	3.23E-05	0.5	0.0	1.4	4.79E-05	0.5	0.0	1.1
	NRG	0.00E+00	1.21E-05	4.4			3.20E-05	4.9			4.72E-05	6.6		
	GRS	0.00E+00	9.11E-06	0.3	0.05	3.9	2.46E-05	0.9	0.03	4.5	4.20E-05	2.1	0.03	5.9
Nd-145	UPM	0.00E+00	9.10E-06	0.7	0.0	2.8	2.46E-05	0.5	0.0	1.6	4.18E-05	0.5	0.0	1.1
	NRG	0.00E+00	9.05E-06	4.9			2.48E-05	6.7			4.28E-05	10.9		
	GRS	0.00E+00	7.53E-06	0.3	0.0	4.6	2.35E-05	1.0	0.0	5.2	5.05E-05	2.0	0.0	6.7
Nd-148	UPM	0.00E+00	4.20E-06	0.7	0.0	2.1	1.24E-05	0.5	0.0	1.3	2.45E-05	0.4	0.0	0.9
	NRG	-	-				-				-			
	GRS	0.00E+00	1.76E-06	0.3	0.0	16.5	5.58E-06	0.3	0.0	14.5	1.18E-05	0.4	0.0	13

UPM:  $\Delta N$  due to  $\Delta XS$ ,  $\Delta FYs$  and  $\Delta DD$

GRS:  $\Delta N$  due to  $\Delta XS$ ,  $\Delta FYs$  and  $\Delta DD$

NRG:  $\Delta N$  due to  $\Delta XS+FYs$



		0 GWd/MTU			10 GWd/MTU			30 GWd/MTU			60 GWd/MTU			
		mean	mean	rel. std. dev.	mean	rel. std. dev.	mean	rel. std. dev.	mean	rel. std. dev.	mean	rel. std. dev.		
				$\Delta XS$	$\Delta DD$	$\Delta FYs$			$\Delta XS$	$\Delta DD$	$\Delta FYs$			
Sm-149	UPM	0.00E+00	1.17E-07	14.0	0.0	6.4	1.21E-07	14.3	0.0	5.7	1.05E-07	15.5	0.0	5.1
	NRG	0.00E+00	1.09E-07	11.4	0.0		1.15E-07	10.8	0.3		9.97E-08	11.3	0.3	
	GRS	0.00E+00	2.76E-06	1.7		10.1	9.28E-06	2.0		9.5	1.91E-05	2.5		10.6
Sm-152	UPM	0.00E+00	1.30E-06	1.0	0.0	1.9	3.47E-06	1.2	0.0	1.3	5.26E-06	1.6	0.0	0.9
	NRG	0.00E+00	1.25E-06	16.2			3.47E-06	13.3			5.37E-06	11.7		
	GRS	0.00E+00	2.51E-07	0.8	0.0	15.2	9.61E-07	1.8	0.1	11.3	2.41E-06	2.9	0.1	8.8
Cs-133	UPM	0.00E+00	1.55E-05	0.7	0.0	2.0	4.36E-05	0.5	0.0	1.1	7.63E-05	0.4	0.0	0.9
	NRG	0.00E+00	1.50E-05	3.5			4.25E-05	3.7			7.48E-05	5.4		
	GRS	0.00E+00	4.79E-07	0.2	0.0	3.2	3.72E-06	0.5	0.0	1.7	1.15E-05	1.2	0.0	1.7
Cs-137	UPM	0.00E+00	1.51E-05	0.7	0.1	2.6	4.43E-05	0.5	0.0	1.6	8.59E-05	0.4	0.0	1.2
	NRG	0.00E+00	1.49E-05	2.2			4.42E-05	2.0			8.62E-05	2.1		
	GRS	0.00E+00	1.54E-05	0.0	0.2	1.9	4.47E-05	0.0	0.2	1.7	8.59E-05	0.0	0.2	1.7
Mo-95	UPM	0.00E+00	8.36E-06	1.0	0.0	9.7	3.55E-05	0.7	0.0	6.8	6.90E-05	0.5	0.0	4.8
	NRG	0.00E+00	8.28E-06	4.9			3.56E-05	5.8			6.97E-05	7.6		
	GRS	0.00E+00	1.48E-05	0.1	0.1	5.2	4.15E-05	0.2	0.1	6	7.41E-05	0.4	0.1	7.9
Tc-99	UPM	0.00E+00	1.47E-05	0.7	0.0	2.6	4.15E-05	0.5	0.0	1.6	7.44E-05	0.4	0.0	1.3
	NRG	0.00E+00	1.42E-05	10.4			4.08E-05	9.4			7.39E-05	9.1		
	GRS	0.00E+00	1.29E-05	0.1	0.0	11.2	3.84E-05	0.2	0.01	9.9	7.47E-05	0.4	0.1	9.5

UPM:  $\Delta N$  due to  $\Delta XS$ ,  $\Delta FYs$  and  $\Delta DD$

GRS:  $\Delta N$  due to  $\Delta XS$ ,  $\Delta FYs$  and  $\Delta DD$

NRG:  $\Delta N$  due to  $\Delta XS+FYs$

## IN SHORT

- The **GRS / XSUSA** methodology accounts for **cross-sections and engineering** uncertainties. Now, in addition, it takes into account **fission yields and decay data** uncertainties from ENDF-6 libs.
- Tools to generate pools of varied libraries for **ORIGEN-S** have been developed (**YiSaB** and **DeSaB**) and their outputs are used following the **XSUSA** method of repeated calculations
- The **XSUSA** extended capabilities have been applied to the UAM-6 burnup pincell benchmark.

On k-eff: low impact from decay data uncertainties, Xs main contributors to its uncertainty

On inventory: depending on the nuclide, fission yields and cross-section uncertainties

## FUTURE WORK

- Integration of **YiSaB** and **DeSaB** within the **XSUSA** flow chart so they generate libraries on the fly
- Application of the methodology to complex problems
- **Inclusion of correlations** to be taken into account in the **MEDUSA** sampling of the fission yields (GRS – ORNL collaboration)



**Thank you very much for your attention**

**Questions?**