

# The nuclear data role in the V & V & UQ of Monte Carlo simulations of advanced reactors

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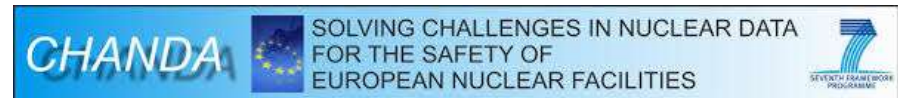
- The capability to provide reliable predictions of Gen-IV reactors recognized as a priority to support the development of those technologies
- High-fidelity neutronics analysis can be performed using 3D Monte Carlo simulations, which involve:
  1. Computer MC codes
  2. Calculation scheme: modeling options
  3. Nuclear data: processing and evaluated libraries
- The most critical input data impacting the quality of MC results are **nuclear data**
- **Verification**, **Validation** and Uncertainty Quantification is required to evaluate the ability of MC simulations to predict the real behavior

## Verification through code benchmarking

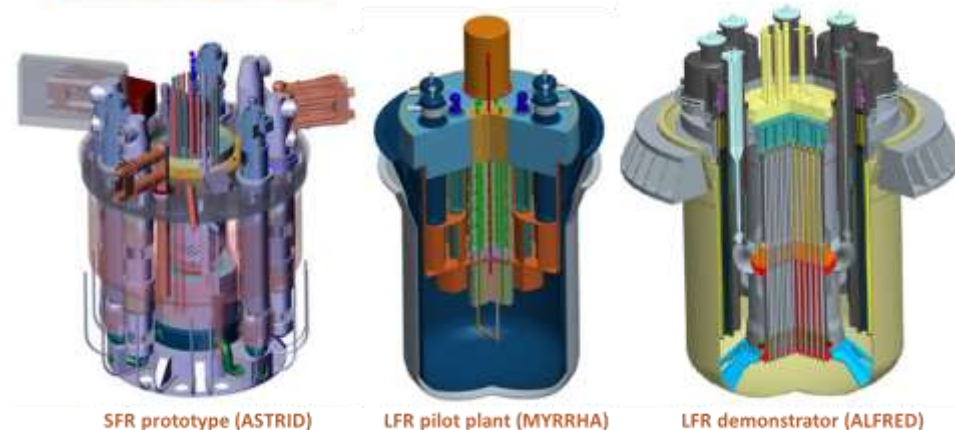
- SCALE6.2 package for evaluation of **fast reactor core performance**
  - KENO-VI Monte Carlo code
  - AMPX-formatted CE ENDF/B-VII.1 based library
- Predicted  $k_{\text{eff}}$  systematically higher (~500 pcm) than the values computed by MCNP and Serpent using the same nuclear data library
- Verification through code benchmarking



**ESFR-SMART**  
sodium fast reactor safety

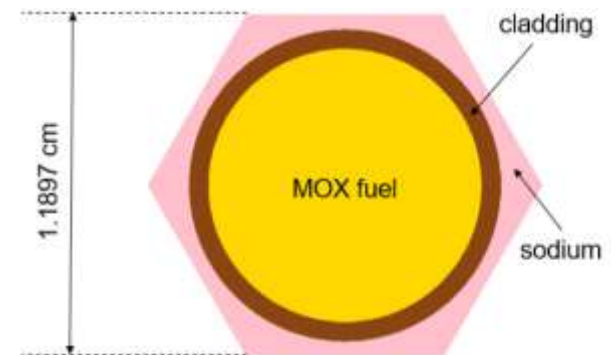


CP+ESFR



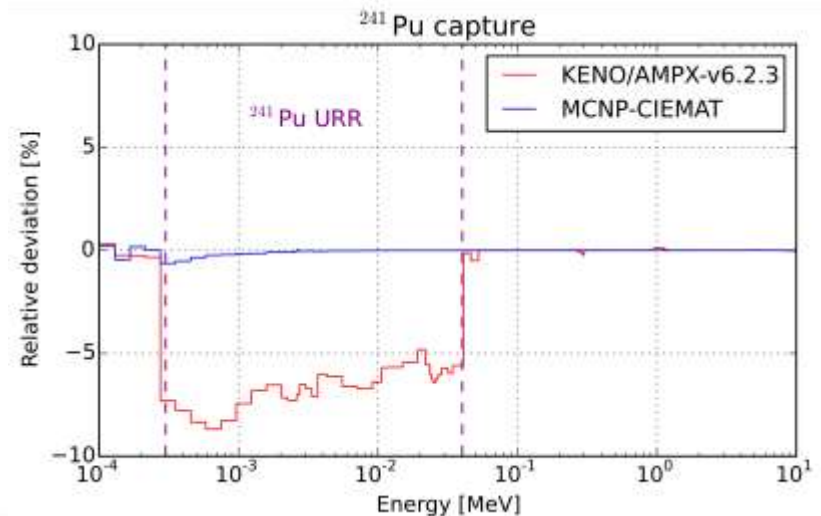
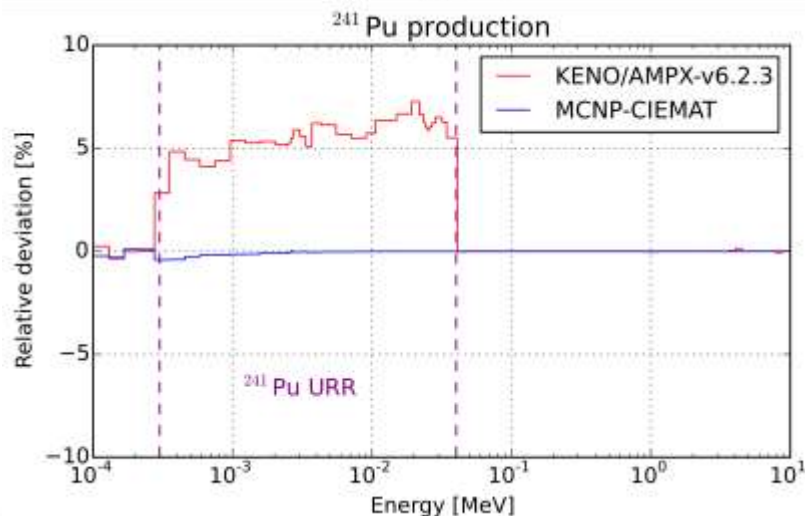
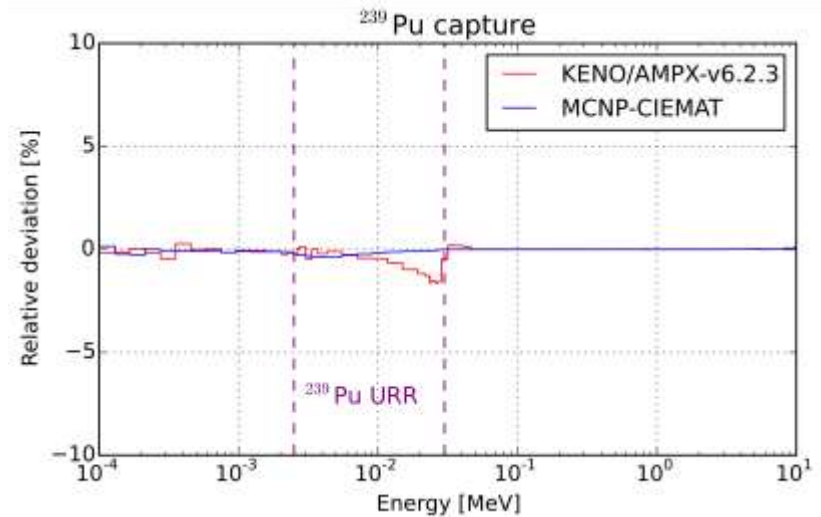
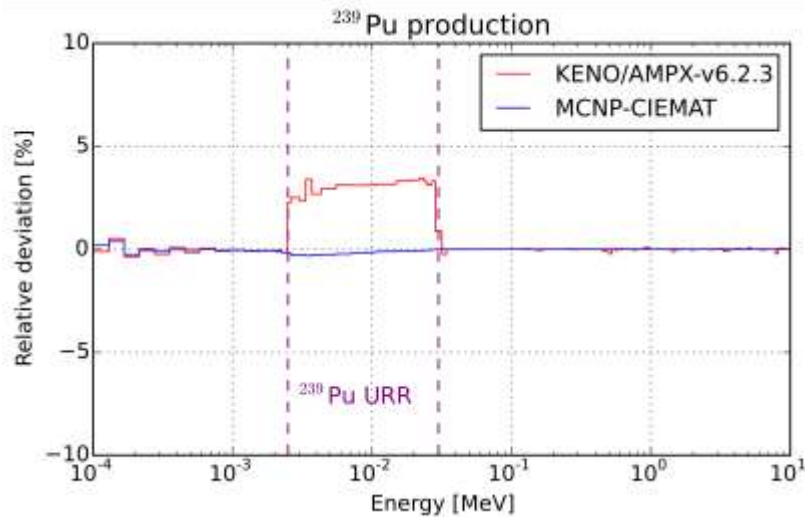
A simplified 2D SFR pin-cell benchmark was launched in order to provide insight into the origin of the discrepancies.

Code	Library	$k_{inf}$ with P-T	$\Delta\rho$ [pcm]
Serpent2	ENDF/B-VII.1 – Serpent	1.31687(2)	<b>reference</b>
MCNP6.1	ENDF/B-VII.1 – Serpent	1.31685(5)	<b>-1</b>
MCNP6.1	ENDF/B-VII.1 – MCNP-6.1	1.31853(5)	<b>96</b>
KENO-VI	ENDF/B-VII.1 – SCALE-6.2.3	1.32607(2)	<b>527</b>



**About the impact of the Unresolved Resonance Region in Monte Carlo simulations of Sodium Fast Reactors**, A. Jiménez-Carrascosa, E. Fridman, N. García-Herranz, F. Alvarez-Velarde, P. Romojaro, F. Bostelmann  
ICAPP 2019

Pu-239 and Pu-241 capture and production reactions were identified as major contributors via one-group collapsed cross section comparison. A detailed comparison reveals an important effect of the unresolved resonance region.



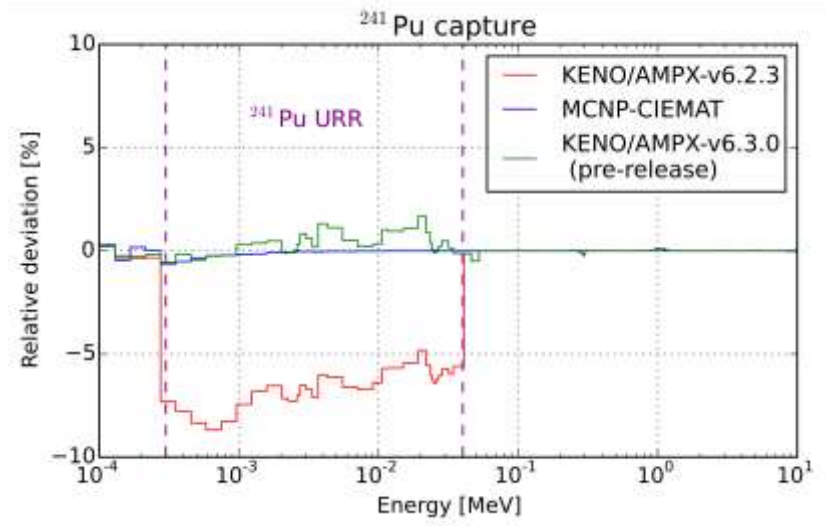
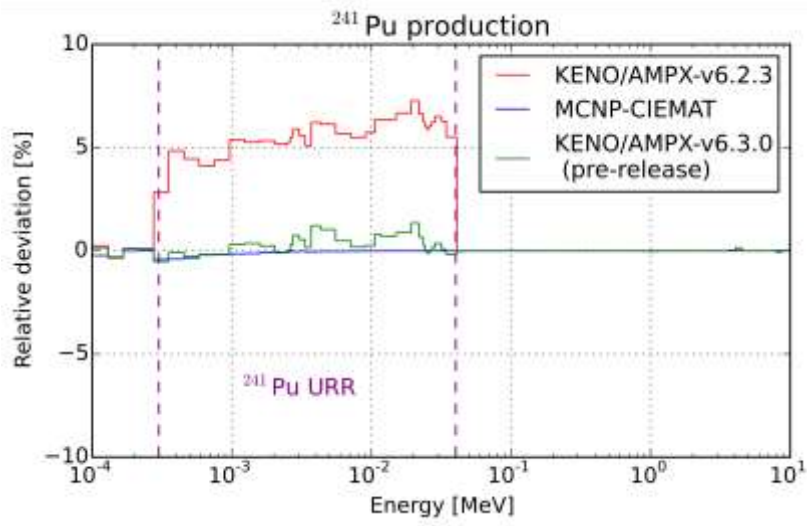
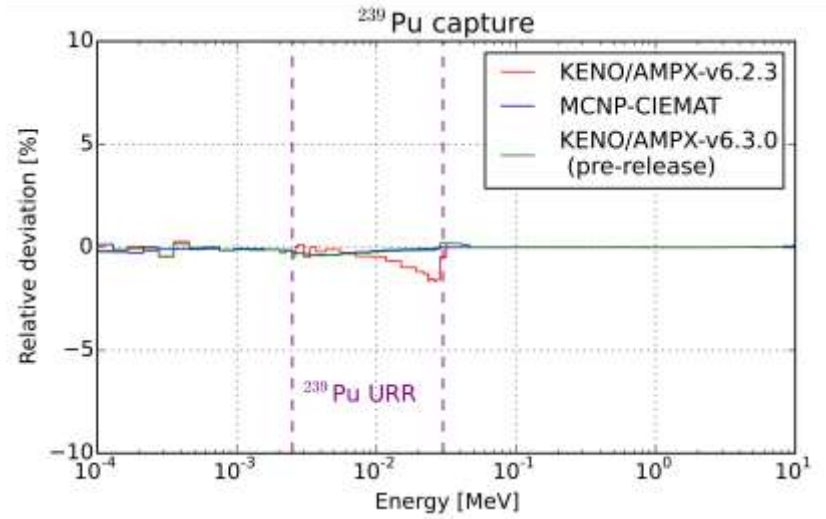
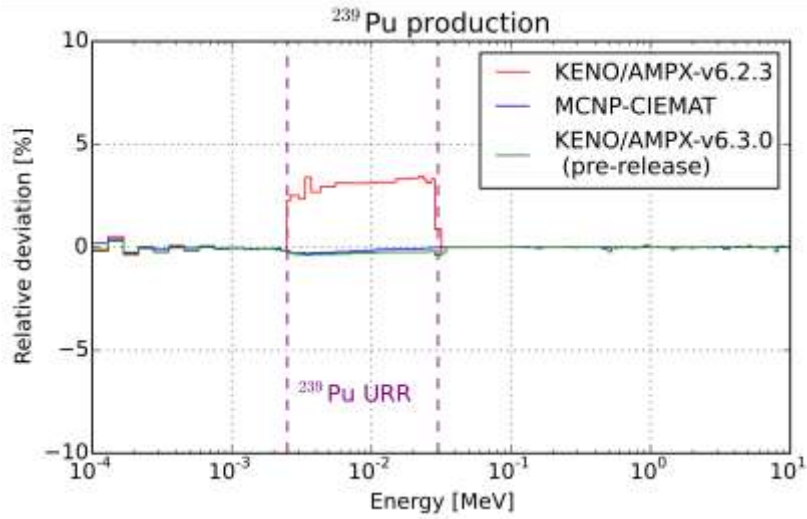
Since KENO-VI overestimates the production cross section and underestimates capture in the URR, the effect of URR in k-eff is highly overestimated with respect to MCNP and Serpent

Code	Library	$k_{inf}$ with P-T	$k_{inf}$ without P-T	URR effect $\Delta\rho$ [pcm]
Serpent2	ENDF/B-VII.1 – Serpent	1.31687(2)	1.31601(2)	<b>50</b>
MCNP-6.1	ENDF/B-VII.1 – Serpent	1.31685(5)	1.31599(5)	<b>50</b>
MCNP-6.1	ENDF/B-VII.1 – MCNP-6.1	1.31853(5)	1.31683(5)	<b>98</b>
KENO-VI	ENDF/B-VII.1 – SCALE-6.2.3	1.32607(2)	1.31689(2)	<b>525</b>

This issue is related with nuclear data processing AMPX code. It has recently been fixed by SCALE Team in the next SCALE release (6.3.0). In this work, SCALE Team tested the corrected library for this benchmark.

KENO-VI	ENDF/B-VII.1 – SCALE-6.3.0	1.31838(2)	1.31689(2)	<b>86</b>
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The improvement can be noticeably seen when using the updated library

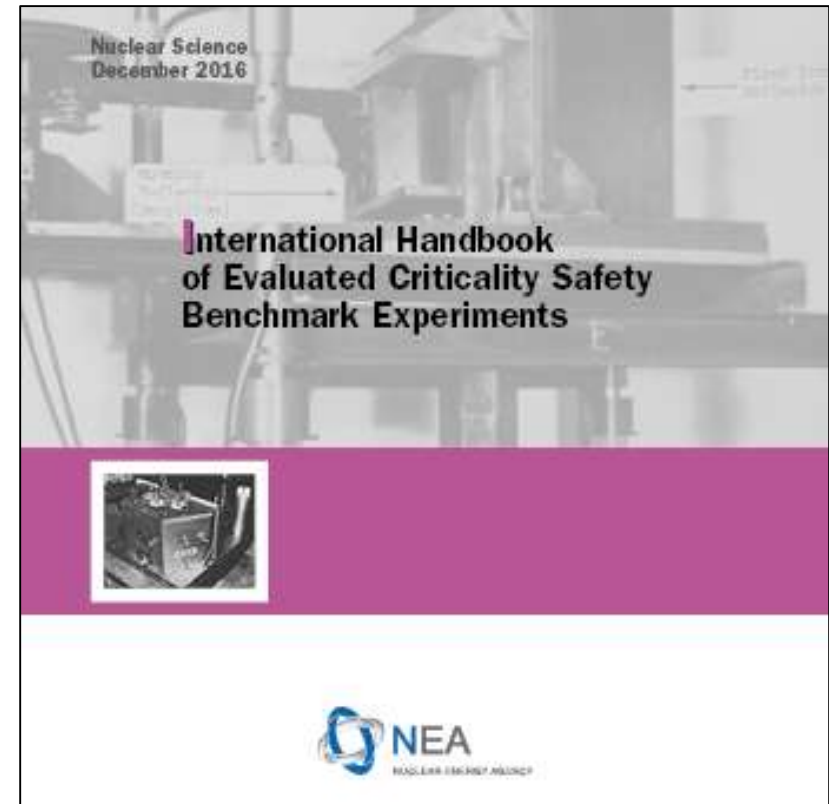


## Verification through code benchmarking - conclusion

- Predicted  $k$ -eff values of fast reactors very sensitive to the treatment of nuclear data in the URR
- Nuclear data processing plays an important role in V&V of MC simulations
- Further analysis required to make recommendations about how to qualify the processed CE libraries before their use in practical applications

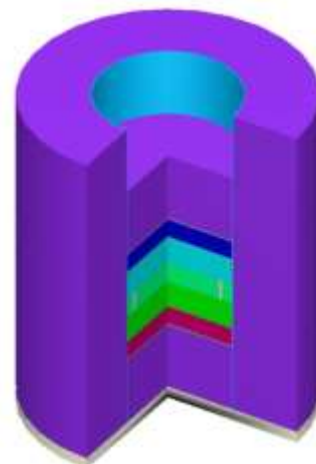
## Verification & Validation against experiments

- Identification of ICSBEP experiments to support validation of MC codes and associated databases in the URR
- A variety of U and Pu benchmarks\* were modeled for KENO-VI in CE (ENDF/B-VII.1)
  - Inputs available in DICE; most of them for MMK-KENO with the ABBN-299 library developed by IPPE (Russia)

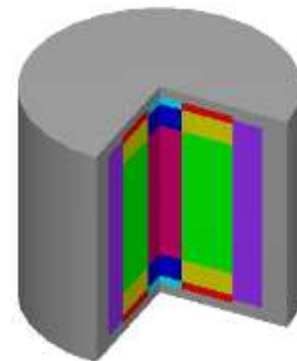


\* **Impact of MCNP unresolved resonance probability-table treatment on Uranium and Plutonium benchmarks**, R.D. Mosteller and R.C. Little, LANL, 6<sup>th</sup> Int. Conf. on Nuclear Criticality Safety, Versailles, France, 1999

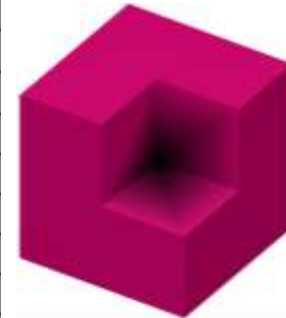
Benchmark name	Case	$k_{eff}$			$\Delta k_{eff}$ (pcm)
		Experimental	with P-T	without P-T	
HEU-COMP-INTER-003	-001	1,00000	1,00705	1,00841	<b>135</b>
	-002	1,00000	1,02931	1,03030	99
	-003	1,00000	0,99579	0,99673	94
	-004	1,00000	1,00325	1,00424	99
	-005	1,00000	0,99751	0,99775	24
	-006	1,00000	0,99848	0,99935	87
	-007	1,00000	0,99433	0,99518	85
HEU-COMP-INTER-004	-001	1,00000	1,01192	1,01188	-5
HEU-MET-FAST-001	-001	1,00000	0,99982	1,00002	20
HEU-MET-INTER-006	-001	0,99770	0,99347	0,99417	70
	-002	1,00010	0,99992	1,00040	48
	-003	1,00150	1,00085	1,00168	82
	-004	1,00160	1,00561	1,00641	80
HEU-SOL-THERM-013	-001	1,00120	0,99837	0,99852	14
	-002	1,00070	0,99770	0,99771	1
	-003	1,00090	0,99411	0,99422	11
	-004	1,00030	0,99580	0,99582	2



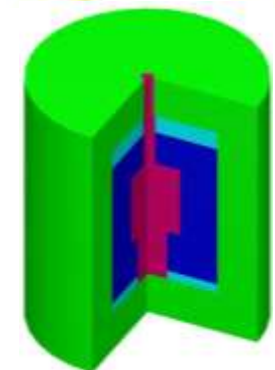
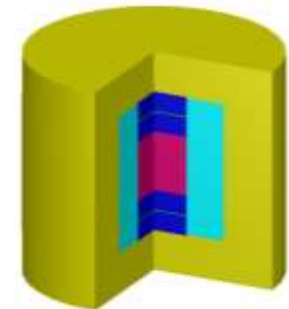
Benchmark name	Case	$k_{eff}$			$\Delta k_{eff}$ (pcm)
		Experimental	with P-T	without P-T	
MIX-COMP-FAST-001	-	0,98660	0,99074	0,98506	<b>569</b>



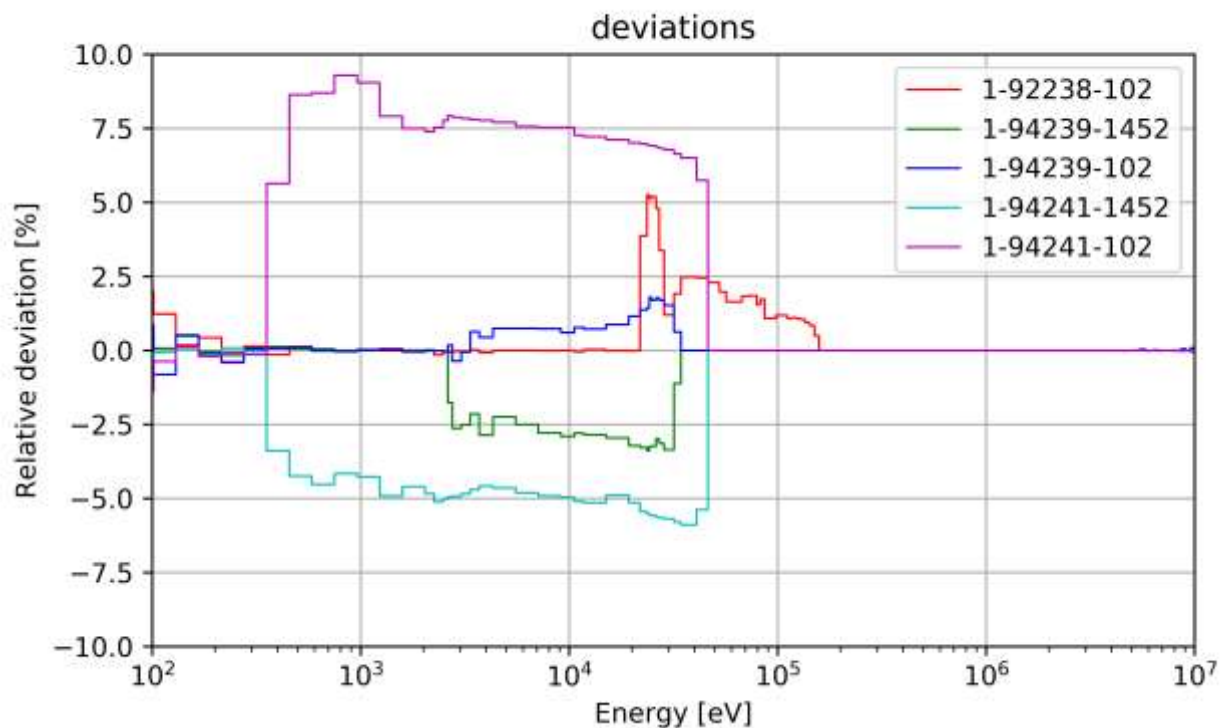
Benchmark name	Case	$k_{eff}$			$\Delta k_{eff}$ (pcm)
		Experimental	with P-T	without P-T	
PU-COMP-INTER-001	-001	1,00000	1,012974	1,011745	<b>-123</b>
PU-MET-FAST-001	-001	1,00000	1,001089	1,000962	-13
PU-MET-FAST-002	-001	1,00000	1,000251	1,000364	11
PU-SOL-THERM-021	-001	1,00000	1,004893	1,004999	11
	-002	1,00000	1,004977	1,005201	22
	-003	1,00000	1,004490	1,004590	10
	-004	1,00000	0,369916	0,369973	6
	-005	1,00000	1,004632	1,004635	0,3
	-006	1,00000	1,006951	1,007089	14



Benchmark name	Case	$k_{eff}$			$\Delta k_{eff}$ (pcm)
		Experimental	with P-T	without P-T	
IEU-COMP-FAST-004	-	0,99780	1,00039	0,99820	<b>-219</b>
IEU-MET-FAST-004	DET	1,00000	1,00771	1,00789	18
	SIM	1,00000	1,00735	1,00786	51
IEU-MET-FAST-007	DET	1,00490	1,14433	1,14433	0,4
	SIM	1,00450	1,00530	1,00072	<b>-458</b>
LEU-SOL-THERM-001	-001	0,99910	1,01145	1,01123	-22



## Example of cross-section deviations for MIX-COMP-FAST-001



Development of a script for an automatized analysis of the URR effect based on comparison of cross-sections with and without PT

## Verification and validation against experiments - conclusion

- Comparison of KENO-VI results with and without PT in the URR allows identify the most sensitive configurations to URR
  - Configurations recommended to qualify the AMPX-processed CE libraries before their use in MC transport codes for practical applications to fast reactors
    - Selected benchmarks and materials (ongoing work)
      - MIX-COMP-FAST-001, IEU-COMP-FAST-004, IEU-MET-FAST-007, HEU-COMP-INTER-003-001, PU-COMP-INTER-001
  - Validation will be addressed after the released of SCALE6.3
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- Processing of nuclear data can be an important source of errors in MC transport calculations of fast reactors
  - Verification & Validation of the processed continuous-energy libraries is required before their use for fast reactor applications

# Thank you for your attention!

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I Jornada CEIDEN de usuarios de bases de datos nucleares | 7 Mayo 2019