

# Assessing and Enhancing SCALE Capabilities to Model Fast Neutron Spectrum Systems

Generation of AMPX MG libraries for fast reactor systems

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### Outline

- Motivation and models of interest
- Generation of new AMPX MG libraries
- First results of criticality calculations
- First results of uncertainty calculations
- Summary and future work
- Acknowledgements



# 1. Motivation and models of interest

Why do we need another AMPX MG library for the analysis of fast reactor systems with SCALE?



#### Flux spectrum of typical LWR and SFR systems



Possible MG libraries in SCALE 6.2:

- 252g ENDF/B-VII.1
- 999g ENDF/B-VII.1



#### Investigated models: homogenized fuel assemblies

- Homogenization to avoid geometrical effects on results
- Metallic fuel of MET1000:
  - 1000 MWth Advanced Burner Reactor
  - Proposed within the UAM SFR benchmark
  - Metallic driver fuel of the inner core zone
  - BOEC fuel: U/Pu/MA (U/TRU)
- Oxide fuel of MOX3600:
  - 3600MWth large oxide core
  - Proposed within the UAM SFR benchmark
  - Oxide driver fuel of the inner core zone
  - BOEC fuel: U/Pu/MA (U/TRU)





#### **Utilized Codes**

- Reference: KENO-CE (SCALE 6.2)
- Investigation of new MG libraries: T-NEWT (SCALE 6.2)





#### Comparison of KENO-CE and T-NEWT with the 252g library – MET1000





#### **Comparison of the eigenvalues**

	KENO-CE	T-NEWT 252g v7.1	T-NEWT 999g v7.1
MET1000	1.29389	1.28979 (-410 pcm)	1.29228 (-161 pcm)
MOX3600	1.19374	1.19699 (325 pcm)	1.19364 (-10 pcm)

- The 252g library does not work well for the investigated fuel types
- The 999g library shows reasonable agreement; however, it is not an option for uncertainty calculations due to the long runtime
- We need another group structure for fast systems!



# 3. Generation of new AMPX MG libraries



#### MG structure and weighting spectrum

- Find suitable MG structure:
  - ANL group structures: 230g, 425g, 2082g
  - Based on 2082 equal lethargy bins between 0.414 eV and 14.191 MeV
  - Fine resolution for fast energies
  - E.g. only 13 groups up to 5 eV in 230g/425g structure compared to almost 100 in the 252g structure
- Find best weighting spectrum for the generation of MG cross sections:
  - Watt fission spectrum of Pu-239
  - Weighting spectra generated with CENTRM using the investigated homogenized fuel assemblies (MET1000, MOX3600)



#### **Considered weighting spectra**





# 4. First results of criticality calculations



#### First comparison with 230g structure – MET1000





#### First comparison with 230g structure – MET1000





#### First comparison with 230g structure – MET1000





#### Influence of different weighting spectra – MET1000





## **Overview of MET1000 (U/TRU) calculations**

		k-inf	Δk [pcm]
KENO-CE	ENDF/B-VII.1	1.29389(10)	(ref)
T-NEWT	252g v7.1	1.28979	-410
T-NEWT	999g v7.1	1.29228	-161
T-NEWT	230g v7.1 – watt	1.29383	-6
T-NEWT	230g v7.1 – met1000	1.29547	-158
T-NEWT	425g v7.1 – watt	1.29248	-141
T-NEWT	2082g v7.1 – watt	1.29252	-137



## **Overview of MOX3600 (U/TRU) calculations**

		k-inf	Δk [pcm]
KENO-CE	ENDF/B-VII.1	1.19374(11)	(ref)
T-NEWT	252g v7.1	1.19699	325
T-NEWT	999g v7.1	1.19364	-10
T-NEWT	230g v7.1 – watt	1.19576	202
T-NEWT	230g v7.1 – mox3600	1.19526	152
T-NEWT	245g v7.1 – watt	1.19486	113
T-NEWT	245g v7.1 – mox3600	1.19455	81
T-NEWT	253g v7.1 – mox3600	1.19423	49
T-NEWT	425g v7.1 – watt	1.19376	3
T-NEWT	2082g v7.1 – watt	1.19362	-12



# 5. First results of uncertainty calculations



#### **Uncertainty analysis**

- Requirements:
  - Generation of 230g covariance library
  - Weighting function: watt fission spectrum
  - Reference for uncertainty calculations: TSUNAMI-CE calculations



## **Uncertainty analysis of MET1000**

	XS lib	Cov lib	%	∆(% ∆k/k)
TSUNAMI-CE	ENDF/B-VII.1	56g	1.4352(12)	(ref)
TSUNAMI-CE	ENDF/B-VII.1	230g	1.4358(12)	0.0006
TSUNAMI-MG*	230g v7.1 - watt	230g	1.4308(6)	-0.0044
TSUNAMI-MG*	230g v7.1 – met1000	230g	1.4285(6)	-0.0067
TSUNAMI-MG*	425g v7.1 - watt	230g	1.4345(4)	-0.0007

\*meaning TSUNAMI-3D-K6 with MG

 $\rightarrow$  Simplified group structure for covariance data might be sufficient



## **Uncertainty analysis of MET1000**

Top contributors to the uncertainty in k-inf:

nuclid	cova e-reaction	% Δk/k due to this matrix		
u-238	n,n'	u-238	n,n'	1.2053(9)
na-23	elastic	na-23	elastic	0.3242(2)
fe-56	elastic	fe-56	elastic	0.2590(3)
u-238	n,gamma	u-238	n,gamma	0.2435(1)
fe-56	n <i>,</i> n'	fe-56	n,n'	0.2388(1)



#### Sensitivities as a function of energy – U-238 n,n'





#### Sensitivities as a function of energy – Pu-239 nubar





# 6. Summary and future work



### Summary

- The present fine-group cross section libraries are not optimal for fast systems
- A 230g structure with watt fission spectrum as weighting function generates reasonable agreement with reference in criticality and uncertainty calculations
- Results with 425g and 2082g are similar; a finer groups structure might therefore not be necessary
- Group structure of the covariance data has minor influence on uncertainty result



#### **Future work**

- 1) Generation of few-group xs with TRITON for use in nodal codes and 2) uncertainty calculations:
  - different fine-group libraries
  - homogeneous vs. heterogeneous fuel assemblies
  - different super-cells
  - leakage correction via B1 method
- Investigation of simplified group structure of covariance data on uncertainty quantification
- Systematic uncertainty analyses (fuel pin, assembly, full core)
- Calculation of full cores of the UAM SFR benchmark







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#### Comparison of KENO-CE and T-NEWT with the 252g library – MET1000





## Investigated models – MET1000





# Influence of upper boundary of PW range in self-shielding calculation – MET1000





Influence of upper boundary of PW range in self-shielding calculation – MET1000





#### Influence of self-shielding factors in URR – MET1000

- Bondarenko shielding factors for the 238g library were computed using an analytical approximation for the flux spectrum
- In the unresolved resonance range, self-shielding factors were calculated using probability tables for the 252g library

230g, watt, with ptables	∆k=-6 pcm
230g, watt, w/o ptables	Δk=-258 pcm



#### **Difference between KENO-CE, Serpent and MCC-3 – MET1000**

10 <sup>0</sup> 10 <sup>-1</sup> 10 <sup>-2</sup> 10 <sup>-3</sup> 10 <sup>-4</sup>	keno-ce serpent mcc-3		for the second s	rydloddor y			
10 <sup>-6</sup>						k-inf	∆k [pcm]
10 <sup>-8</sup>				0.11.0	KENO-CE	1.29350(11)	(ref)
10 <sup>-9</sup> 10		10 <sup>3</sup>	10 <sup>4</sup> 10	℃ DF/B-\	Serpent/MCNP	1.28750(9)	-600.0
			Energy [eV]	ENI	MCC-3	1.28894	-456.0
				1.1 1.1	KENO-CE	1.29389(10)	(ref)



#### **Difference between KENO-CE and Serpent – MET1000**

Full core calculations:



		k-inf	∆k [pcm]
ENDF/B- VII.0	KENO-CE	1.04089(5)	(ref)
	Serpent	1.03771(5)	-318
1.1 I.1	KENO-CE	1.03928(5)	(ref)*
END	Serpent	1.03638(5)	-290*

\* Without ptables: agreement



#### Takeaways

- MET1000 (U/TRU):
  - The 230g library leads to good agreement with the reference
  - Influence of weighting spectrum is small regarding the flux spectrum; however, clearly noticeable regarding k-inf
  - Impact of different approach for Bondarenko factors in the URR region confirmed
  - Upper boundary of PW flux calculation should be raised up to 100KeV
  - Significant difference between KENO-CE and MCNP/Serpent due to differences in probability tables
  - More groups lead to larger disagreement regarding k-inf
- MOX3600 (U/TRU):
  - 425g library shows best agreement
  - Reasonable agreement can be obtained with 253g