

Recent R&D Activities at NCSU using SCALE Tools

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Overview

- The SCALE package has been extensively used in the Nuclear Engineering Department (NED) at North Carolina State University (NCSU)

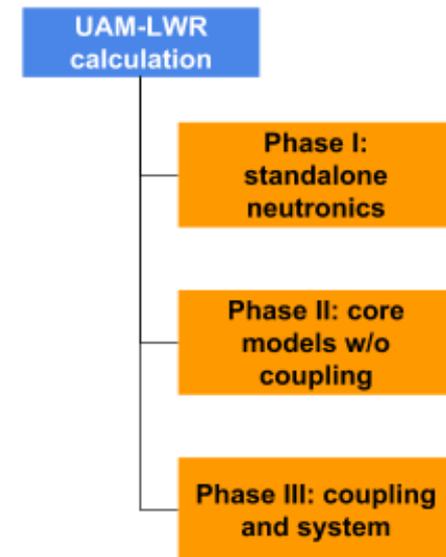
- Research activities:
 - Sensitivity analysis (SA) and uncertainty quantification (UQ) in modeling and simulation of reactors
 - Development of multi-physics and multi-scale reactor analysis platform

- Curriculum activities:
 - Senior design projects
 - Course projects in graduate classes

- This presentation intends to give an overview of various activities since last workshop:
 - Primarily focusing on activities in the Reactor Dynamics and Fuel Modeling Group (RDFMG), which is part of NED, NCSU

OECD/NEA LWR Uncertainty Analysis in Modeling (UAM) Benchmark

- Overview:
 - Aims to test consistently uncertainty propagation from basic data and engineering uncertainties across different scales (multi-scale) and physics phenomena (multi-physics)
 - In three phases consisting of ten benchmark exercises
 - On a number of numerical and experimental test cases
- Phase I (Neutronics Phase) – **completed**:
 - Exercise I-1: Cell Physics
 - Exercise I-2: Lattice Physics
 - Exercise I-3: Core Physics
- Phase II (Core Phase) – **ongoing**:
 - Exercise II-1: Fuel Physics
 - Exercise II-2: Time Dependent Neutronics
 - Exercise II-3: Bundle Thermal-Hydraulics
- Phase III (System Phase) – **ongoing**:
 - Exercise III-1: Core Multi-Physics
 - Exercise III-2: System Thermal-Hydraulics
 - Exercise III-3: Coupled Core-System
 - Exercise III-4: Comparison of BEPU vs. Conservative Calculations



SCALE tools and data used in Phase I

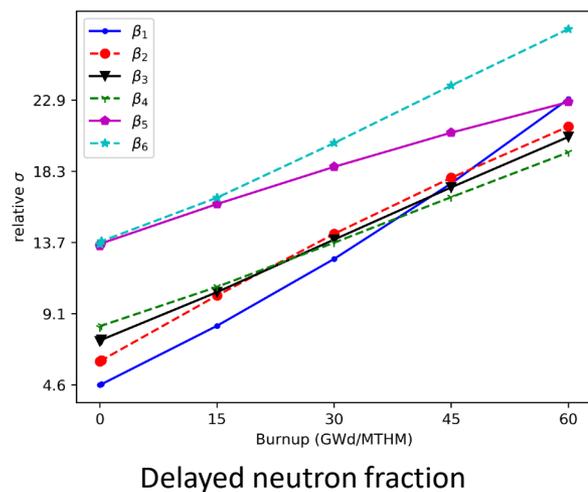
- SCALE lattice physics codes and nuclear data covariance libraries are widely adopted by the participants of LWR UAM benchmark:
 - 19 results (~ 39%) used SCALE solvers, i.e., Polaris & NEWT
 - 36 results (~75%) used SCALE covariance libraries provided in various versions (5.1, 6.0, 6.1 or 6.2)
 - Both SAMPLER (sampling approach) and TSUNAMI (deterministic approach) are widely used for uncertainty propagation

- SCALE covariance libraries
 - A range of different tests (e.g., critical benchmark experiments) are performed to investigate and adjust the new covariance data from evaluated nuclear data libraries
 - Produces more realistic estimate of the uncertainty of integral parameters due to nuclear data uncertainty

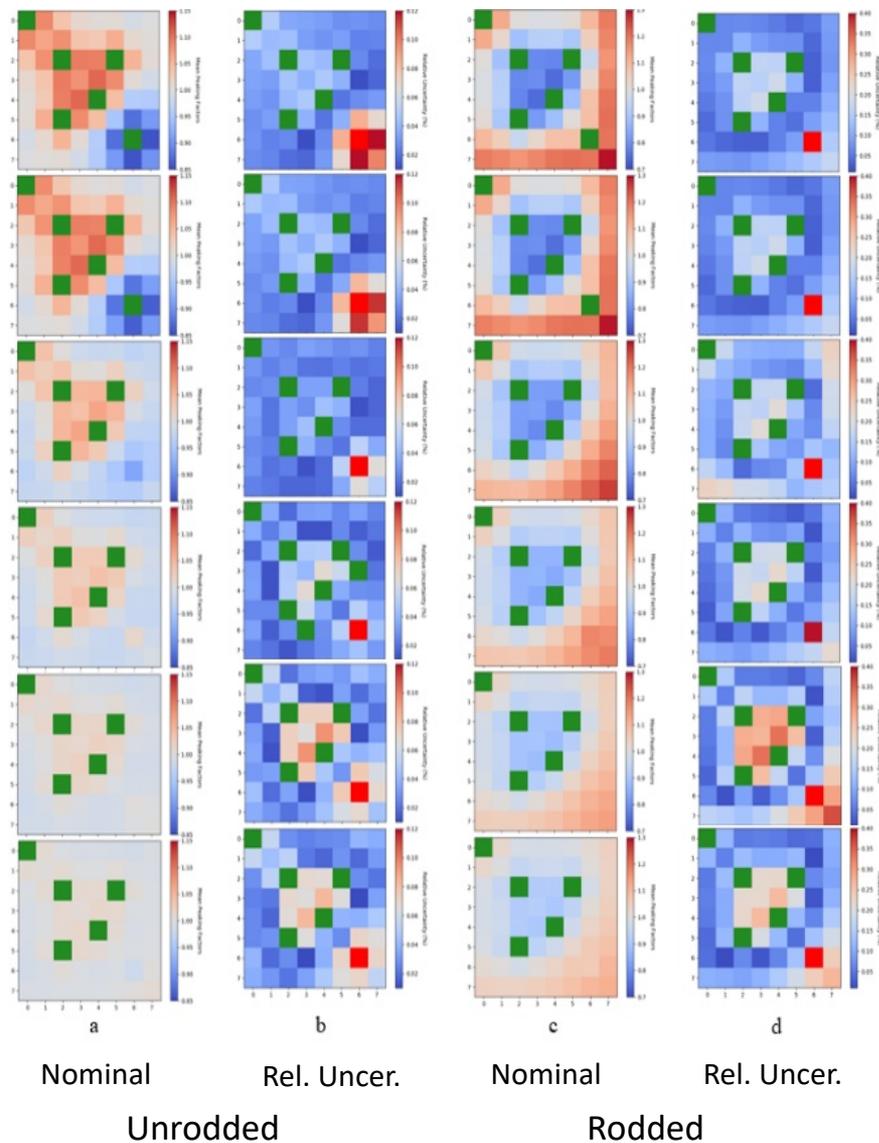
Case	NDL	Transport Code	VCN	UQ Method
1	ENDF/B-VI	SERPENT 2	SCALE 6.0	Deterministic
2	ENDF/B-V	SCALE 6.0	SCALE 6.0	Deterministic
3	ENDF/B-VI	MULTICELL	SCALE 5.1	Sampling
4	ENDF/B-VI	MULTICELL	SCALE 5.1	Sampling
5	ENDF/B-VI	KIKO3D	SCALE 5.1	Sampling
6	ENDF/B-VII.0	XSDRNPM	SCALE 6.1	Deterministic
7	ENDF/B-VI	CASMO-4	SCALE 6.0	Deterministic
8	ENDF/B-VII.RO	CASMO-5MX	SCALE 6.0	Sampling
9	ENDF/B-VII.0	NEWT	SCALE 6.1	Deterministic
10	ENDF/B-VI	MGRAC	SCALE 6.1	Sampling
11	ENDF/B-VII	MCNP5	SCALE 6.0	Deterministic
12	ENDF/B-VII.0	NEWT	SCALE 6.1	Deterministic
13	ENDF/B-VII.0	NEWT	SCALE 6.2	Sampling
14	ENDF/B-VII.1	COBAYA	SCALE 6.2	Sampling
15	ENDF/B-VII.1	COBAYA	SCALE 6.2	Sampling
16	ENDF/B-VII.1	COBAYA	SCALE 6.2	Sampling
17	ENDF/B-VII.1	COBAYA	SCALE 6.2	Sampling
18	ENDF/B-VII.1	POLARIS	SCALE 6.2	Sampling
19	ENDF/B-VII.1	NEWT	SCALE 6.2	Sampling
20	ENDF/B-VII.0	NEWT	SCALE 6.2	Sampling
21	JENDL-4.0	CASMO5	JENDL-4.0	Sampling
22	ENDF/B-VII.0	NEWT	SCALE 6.2	Deterministic
23	ENDF/B-VII.0	NEWT	SCALE 6.2	Deterministic
24	ENDF/B-VII.0	NEWT	SCALE 6.2	Deterministic
25	ENDF/B-VII.1	McCARD	ENDF/B-VII.1	Deterministic
26	ENDF/B-VII.1	MCS	ENDF/B-VII.1	Deterministic
27	ENDF/B-VII.1	MCS	SCALE 6.1	Deterministic
28	ENDF/B-VII.1	MCS	ENDF/B-VII.1	Deterministic
29	ENDF/B-VII.1	MCS	SCALE 6.1	Deterministic
30	ENDF/B-VII.1	STREAM	SCALE 6.2	Deterministic
31	ENDF/B-VII.1	STREAM	ENDF/B-VII.1	Deterministic
32	ENDF/B-VII.1	STREAM	ENDF/B-VII.1	Sampling
33	ENDF/B-VII.0	NEWT	SCALE 6.1	Deterministic
34	ENDF/B-VII.1	NEWT	SCALE 6.2	Deterministic
35	ENDF/B-VII.1	HELIOS2	SCALE 6.1	Sampling
36	ENDF/B-VII.0	NEWT	SCALE 6.1	Sampling
37	ENDF/B-VII.1	NEWT	SCALE 6.2	Sampling
38	ENDF/B-VI	NEWT	SCALE 6.1	Deterministic
39	JEFF-3.1.2	WIMS	WIMS ¹	Sampling
40	ENDF/B-VII.0	NEWT	SCALE 6.2	Sampling
41	ENDF/B-VII.0	NEWT	SCALE 6.2	Sampling
42	JEFF-3.1.2	WIMS	WIMS ¹	Sampling
43	JEFF-3.1.2	WIMS	WIMS ¹	Sampling
44	JEFF-3.1.2	WIMS	WIMS ¹	Sampling
45	ENDF/B VII.0	RMC	SCALE 6.0	Sampling
46	ENDF/B-VII.1	PARCS	SCALE 6.2	Sampling
47	ENDF/B-VII R1	MPACT	ENDF/B-VII.1	Sampling
48	ENDF/B-VII.1	SCALE 6.0	ENDF/B-VII.1	Sampling

Phase II, Exercise II-2a: TMI-I PWR assembly depletion

- Output uncertainties targeted
 - Fission product concentrations
 - Actinide concentrations
 - Two-group cross sections
 - Delayed neutron data
 - Peaking factors
- POLARIS: lattice physics calculation
- ORIGEN: depletion calculation
- SAMPLER: cross section, fission yield, manufacturing data perturbation

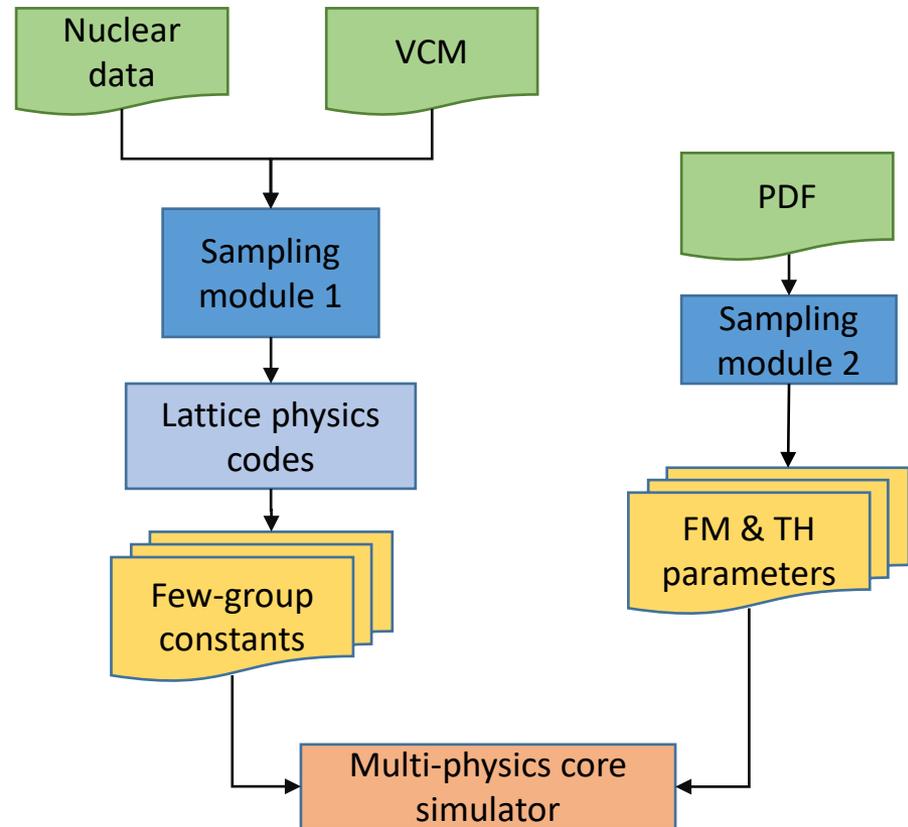


Pin-wise power distribution



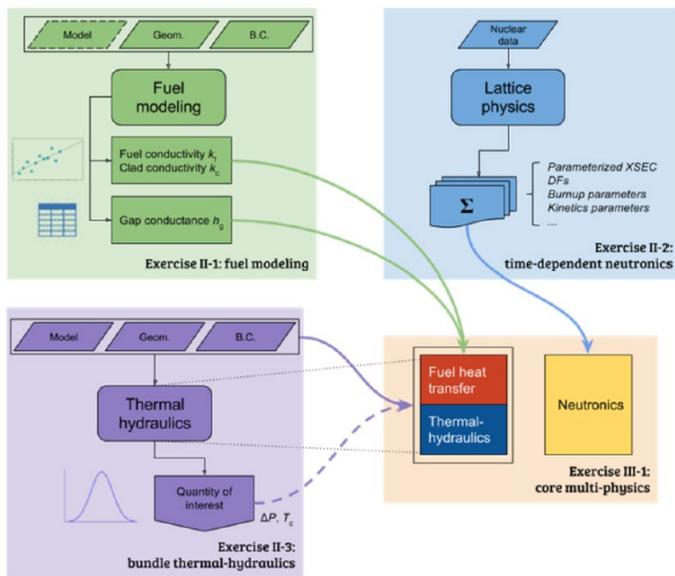
Contribution to Exercise III-1: core multi-physics

- Uncertainty propagation approach for multi-physics core simulation:
 - Compatible with two-step core simulation method
 - Uncertainties from different physics domains (neutronics, thermal-hydraulics, fuel performance) are considered to be *uncorrelated*
- SCALE 6.2 tools were used to prepare perturbed cross section libraries:
 - Sampler: general stochastic sampling method for uncertainty propagation
 - Polaris: new LWR lattice physics neutron transport code

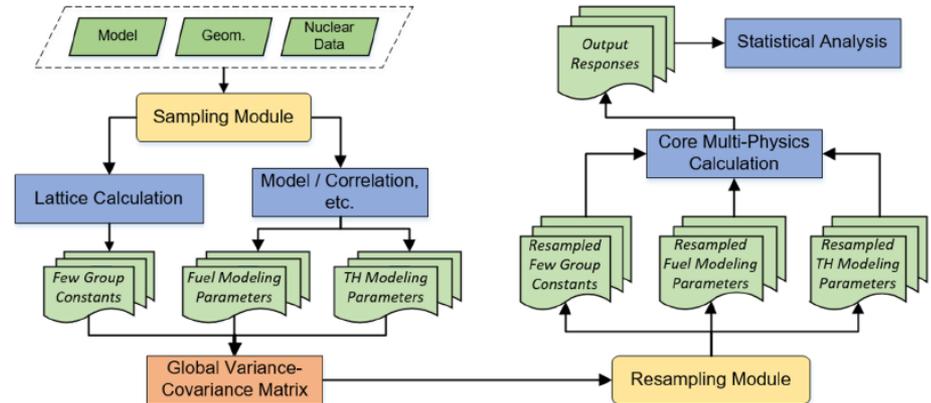


Contribution to Exercise III-1: core multi-physics (cont.)

Problem: Usually multi-physics correlations are not considered



Idea: Estimate a Global Covariance Matrix by propagating common sources uncertainty



PhD dissertation: Development of the consistent uncertainty propagation methodology (K. Zeng)

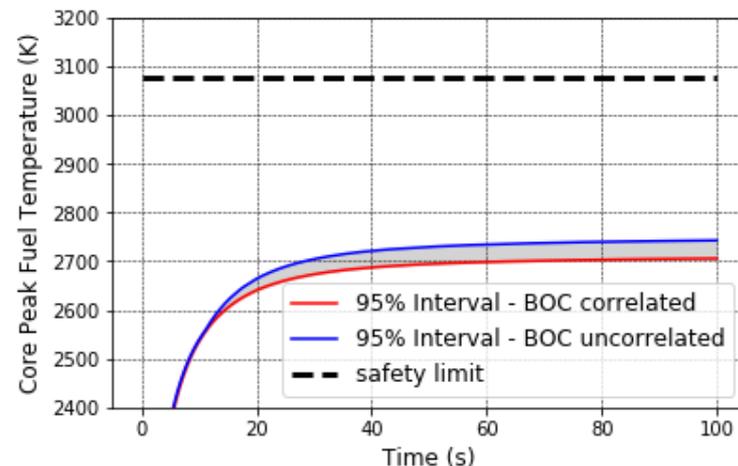
Consistent uncertainty propagation methodology

- Global Covariance Matrix construction
- Application to Exercise III-1 for steady state, depletion and Rod Ejection Accident (REA) in TM-1 core
- Significance: taking into account multi-physics correlations reduces uncertainties and creates larger design margins

Input parameters	Impact			Uncertainty
	NK	TH	FM	
Fuel rod radius R_{fuel}	✓	✓	✓	0.99% (normal)
Gap thickness T_{gap}	✓	✓	✓	5.25% (normal)
Cladding thickness T_{clad}	✓	✓	✓	0.89% (normal)
Fuel rod density ρ_{fuel}	✓		✓	1.65% (normal)
Gadolinia enrichment f_{Gd}	✓		✓	5.43% (normal)
Nuclear cross-sections	✓			SCALE 56-g VCM
System pressure $P_{sys.}$		✓	✓	±1.0% (normal)
Flow rate \dot{m}		✓	✓	±1.5% (normal)
Inlet temperature $\bar{R}_{cool,in}$		✓	✓	±1.0% (uniform)
Total power P		✓	✓	±1.0% (normal)
Power distribution f_{power}	✓	✓	✓	±3.0% (normal)

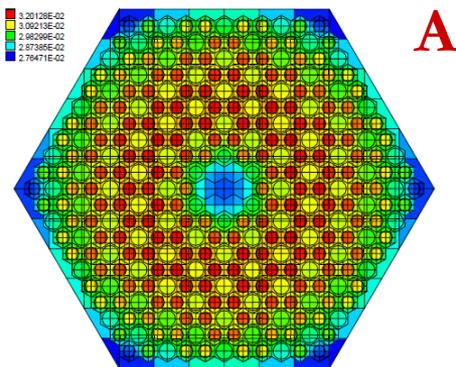
REA results

State	Peak core total power	Peak Fuel Temperature (K)
Uncorrelated BOC	1.71 + 16.3%	2593 + 148
Correlated BOC	1.69 + 17.1%	2598 + 106
Uncorrelated EOC	1.63 + 25.5%	1815 + 95
Correlated EOC	1.65 + 24.3%	1810 + 89

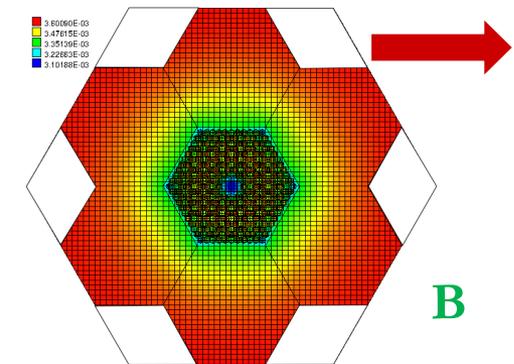


IAEA CRP on HTGR UAM: modeling uncertainty

- To support IAEA CRP High Temperature Gas-cooled Reactor (HTGR) UAM
 - Improve uncertainty modeling in HTGR systems
- Objective: evaluate the cross section sensitivity to the topology of lattice cells after energy collapsing

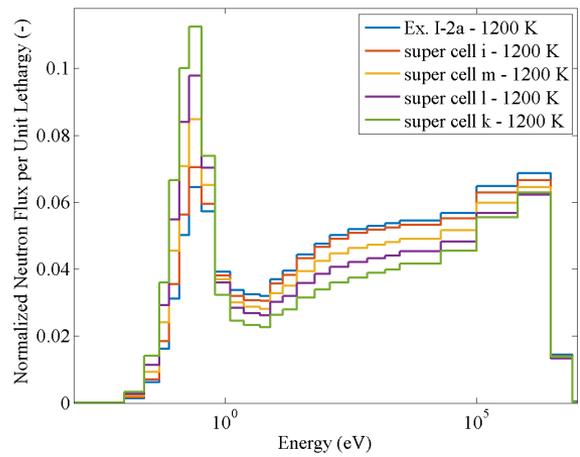


A



B

HTGR super cell



Effect of lattice surroundings on the spectrum (NEWT)

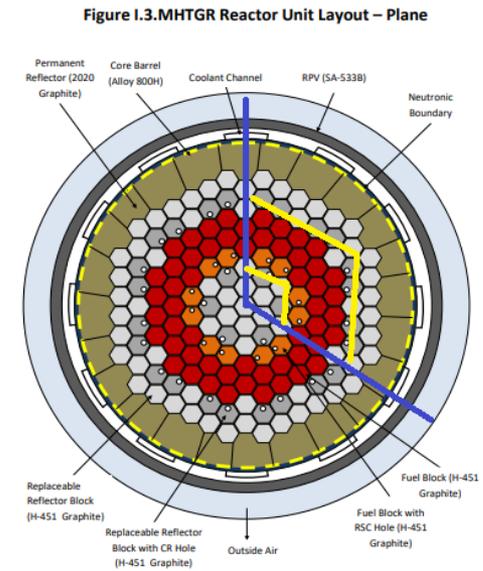
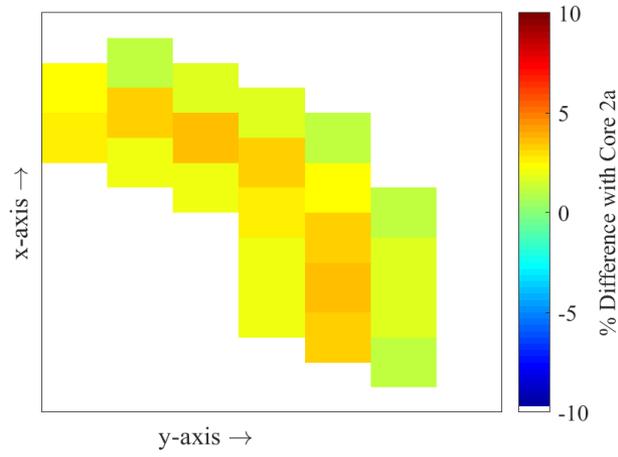


Figure I.3. MHTGR Reactor Unit Layout - Plane

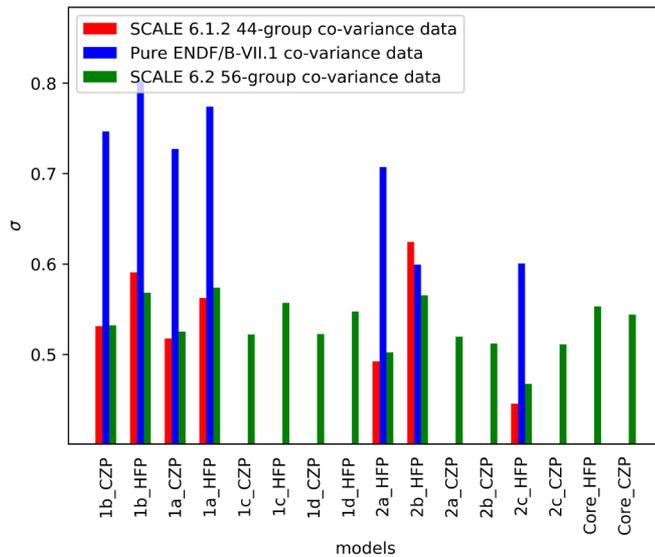


Difference of MHTGR power density between core made of A only and core A+B

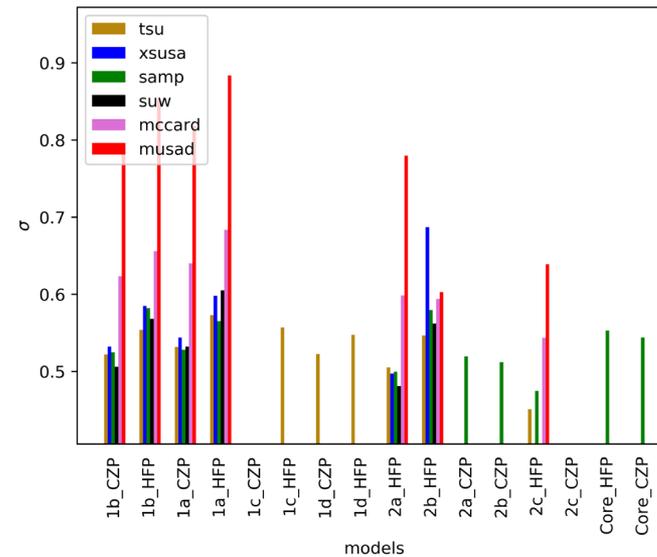
IAEA CRP on HTGR UAM: preparation of final report

Objectives

- Collection and comparative analysis of participants' results obtained throughout the CRP
- The final TecDoc of CRP is expected at the end of the year
- SCALE codes and data were extensively used



k-inf (k-eff) uncertainty based on covariance data

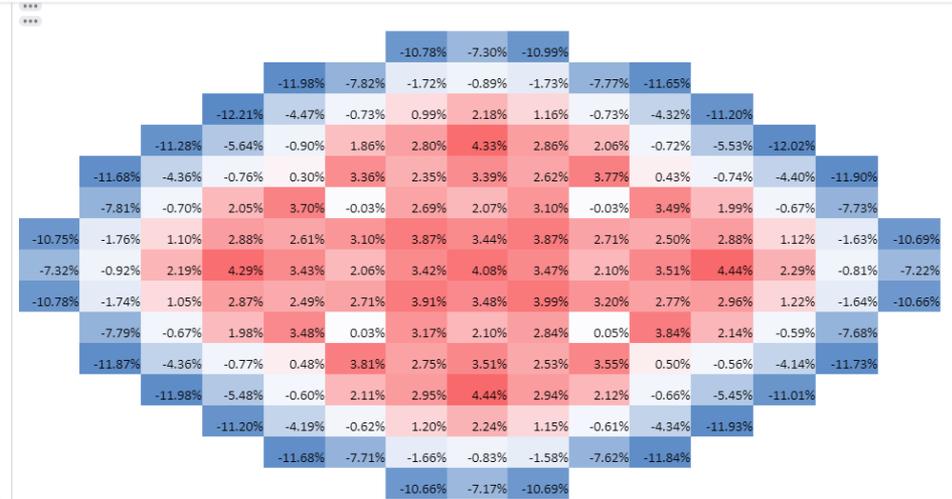
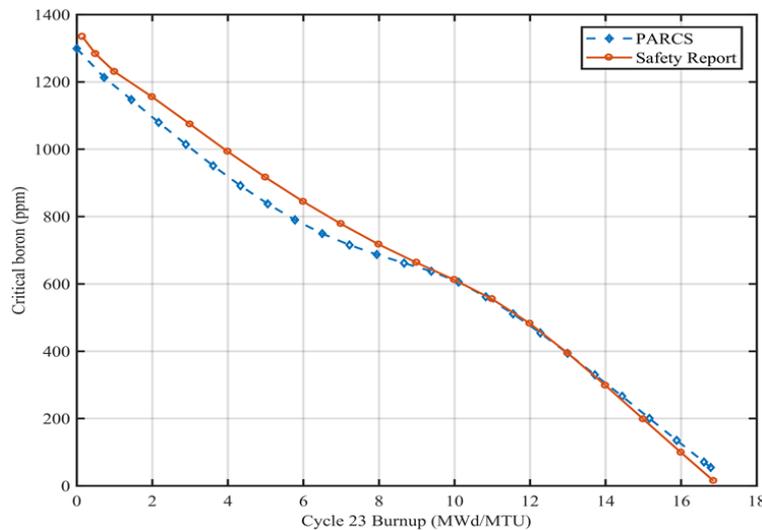


Multi-physics platform for safety analysis based on NRC codes

- Overview
 - Provide training to CNSS (Centre for Nuclear Safety and Security) partners at National Nuclear Regulator (NNR) in South Africa
 - Support Koeberg NPP M&S capability
 - Deliver advanced software capacity based on US NRC codes for safety analysis of LWRs
 - Improved estimates of local parameters
- Software involved: PARCS, CTF, POLARIS, SAMPLER, FRAPTRAN/FRAPCON, TRACE and DAKOTA
- POLARIS used to generate two-group nuclear data on assembly level:
 - Multi-histories libraries
 - Multi-branches libraries
 - Libraries also generated with Serpent for code-to-code comparison
- SAMPLER is used to generate perturbed libraries, on a mono-history, multi-branches level

Multi-physics platform for safety analysis based on NRC codes (cont.)

- Core-level results compared to operational data of Koeberg NPP Cycle 23
- Good agreement with measurement data in initial agreement
 - Central assemblies provide an average RMS of 4.0 % at BOC and 2.1 % at EOC
 - Noticeable differences (~11 %) on the peripheral assemblies - work in progress
 - Perturbed libraries generated

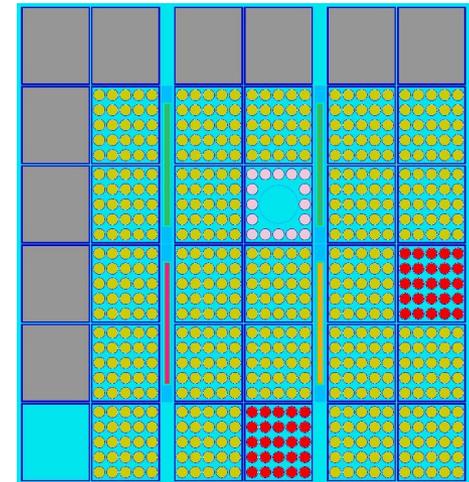


Assembly-wise RMS

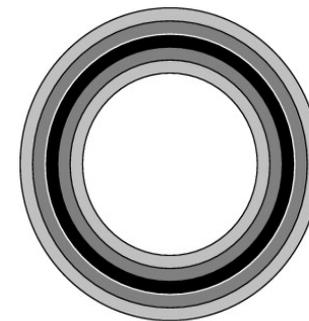
Support to senior design projects

- Molybdenum-99 production in PULSTAR reactor
 - NCSU advisor: Ayman Hawari, Jason Hou
 - ORNL advisor: Ugur Mertuyrek
 - Aims to assess the feasibility of producing Mo-99 in PUSTAR reactor
 - A target containing uranium foil was designed to replace one fuel assembly
 - 3D MC code KENO was used to model reactor core
 - Target design was optimized using the calculated neutron flux and fission rate
 - Safety analysis (RIA, LOCA) was performed to ensure the modified core meets safety limits
 - Economic analysis

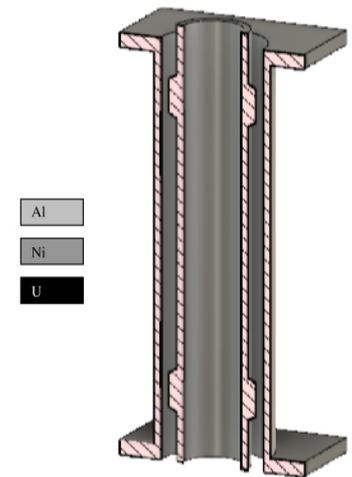
- Prepare undergraduate students for reactor modeling and criticality calculations using state-of-the-art simulation codes



PULSTAR core model
(KENO)



Target design



Target holder model

Summary

- SCALE package has been extensively used in the NED at NCSU to support research and curriculum:
 - Sensitivity analysis (SA) and uncertainty quantification (UQ) in modeling and simulation of reactors
 - NEA/OECD Light Water Reactor (LWR) UAM
 - IAEA CRP High Temperature Gas-cooled Reactor (HTGR) UAM
 - SNF isotopic concentration
 - Development of reactor analysis platform
 - Support to senior design projects
 - Support to course projects in graduate classes such as NE795 “Verification and Validation in Scientific Computing”
- SCALE will be actively utilized also in the following evolving projects at NED, NCSU:
 - Phases II and III of OECD/NEA C5G7-TD benchmark;
 - NEUP project 18-15104 on multi-physics Hi2Lo model information demonstration
 - New NEUP awarded project on “Benchmark Evaluation of Transient Multi-Physics Experimental Data for Pellet Cladding Mechanical Interactions”
 - NEA/OECD Rostov-2 VVER-1000 Multi-Physics Transient Benchmark

Acknowledgements

Main contributors of results presented here:

- NED, NCSU:
 - Postdoctoral scholars: Pascal and Gregory
 - Graduate students: Kaiyue Zeng, Andy Rivas, Khuliso Nevhorwa, Yasemin Ozbek, Cole Takasugi, Quentin Faure, Rofhiwa Tshipuke, Cameron Maras, Chris Gozum
 - Undergraduate students: Jesse Blankenship, Graham Harger, Karthiga Jordan, Scott Burke, Matthew Filer

- We would like to thank the SCALE team for the technical assistance and insightful discussions in the past year, especially:
 - Matt Jessee, Germina Ilas, Will Wieselquist, Ugur Merttyurek