Uncertainty analysis on LWR and HTGR neutronics modeling using SCALE tools at NCSU

Jason Hou

Department of Nuclear Engineering

North Carolina State University

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Oak Ridge National Laboratory

Main contributors of results presented here

- North Carolina State University
  - **Kaiyue Zeng (PhD student)**
  - Jason Hou
  - Kostadin Ivanov

- Tsinghua University
  - **Lidong Wang (PhD student)**
  - Fu Li

- Oak Ridge National Laboratory
  - Matthew Jessee

Reactor Uncertainty Analysis in Modeling (UAM) benchmarks

- Main objectives
  - The chain of uncertainty propagation from basic data, and engineering uncertainties, across different scales (multi-scale), and physics phenomena (multi-physics) to be tested on a number of benchmark exercises for which experimental data is available and for which the power plant details have been released

- The Reactor Dynamics and Fuel Modeling Group (RDFMG) at NCSU has been working on the following Uncertainty Analysis in Modeling (UAM) benchmarks
  - NEA/OECD Light Water Reactor (LWR) UAM
  - IAEA CRP High Temperature Gas-cooled Reactor (HTGR) UAM
  - NEA/OECD Sodium-cooled Fast Reactor (LWR) UAM

- Various modules from different versions of SCALE package have been extensively utilized in support of benchmark specification and calculations
  - Neutronics modeling
  - Sensitivity and uncertainty (S/U) analysis

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NEA/OECD LWR UAM: TMI-1

Kaiyue Zeng, Jason Hou, Kostadin Ivanov

North Carolina State University

Matthew A. Jessee

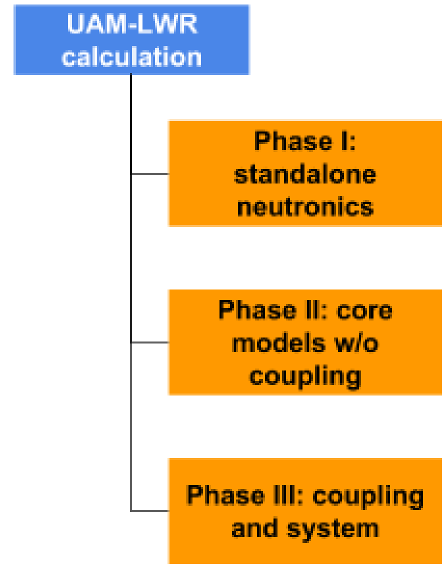
Oak Ridge National Laboratory

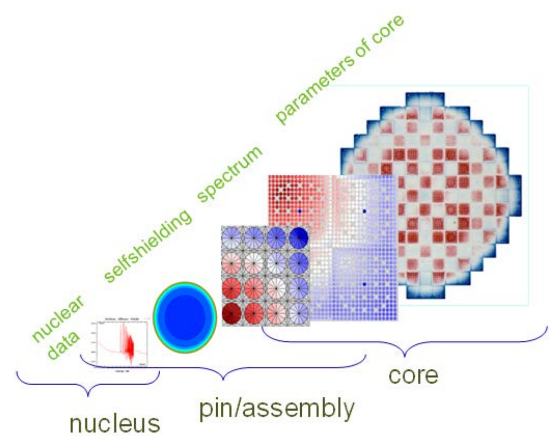
R	4.85 4Gd	4.95 8Gd	4.85 4Gd	A B C				
P	4.85 4Gd CR(6)	5.00 8Gd	4.40 CR(1)	5.00 8Gd	4.95 4Gd+BP			
O	5.00 4Gd+BP	5.00 4Gd CR(5)	5.00 4Gd+BP	4.95 4Gd CR(3)	5.00	5.00 4Gd		
N	4.40 CR(7)	4.95 4Gd+BP	4.95 4Gd APSR(8)	4.95 BP	5.00 4Gd CR(7)	5.00	4.95 4Gd+BP	
M	4.95 4Gd+BP	4.85 4Gd CR(4)	4.95 4Gd+BP	4.40 CR(5)	4.95 BP	4.95 4Gd CR(3)	5.00 8Gd	
L	5.00 4Gd CR(2)	4.95 4Gd+BP	4.95 4Gd CR(6)	4.95 4Gd+BP	4.95 4Gd APSR(8)	5.00 4Gd+BP	4.40 CR(1)	4.85 4Gd
K	4.95 4Gd+BP	4.95 4GD CR(2)	4.95 4Gd+BP	4.85 4Gd CR(4)	4.95 4Gd+BP	5.00 4Gd CR(5)	5.00 8Gd	4.95 8Gd
H	4.00 CR(7)	4.95 4Gd+BP	5.00 4Gd CR(2)	4.95 4Gd+BP	4.40 CR(7)	5.00 4Gd+BP	4.85 4Gd CR(6)	4.85 4Gd
	8	9	10	11	12	13	14	15

A – Fuel enrichment, unit: wt.%
B – Gd and BP pin configuration
C – Control rod type and group number

Uncertainty Analysis in LWR Modeling

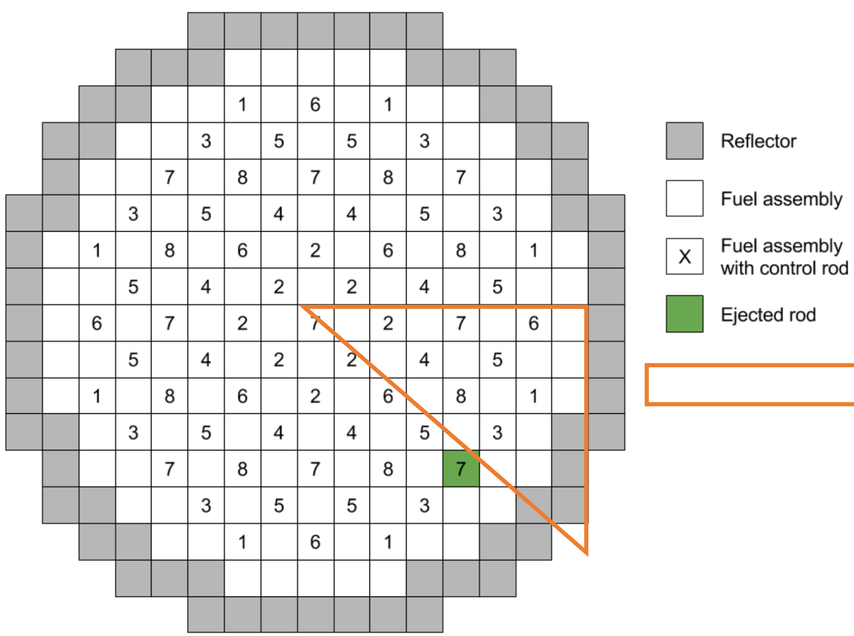
- Objective
  - The work is intended to quantify the uncertainty from nuclear data in the simulation of TMI-1 test cases within the LWR-UAM benchmark framework.
- Exercises
  - Phase I (Neutronics Phase)
    - Exercise I-3: “Core Physics” focused on the core steady-state stand-alone neutronics calculations and their uncertainties.
  - Phase III (System Phase)
    - Exercise III-1: “Coupled Core-System” - Coupled neutronics kinetics thermal-hydraulic core/thermal-hydraulic system performance.





PWR numerical cases based on TMI-1 core design

Parameter	Value	Bank	No. rods	Purpose
Number of fuel assemblies	177	1	8	Safety
Number of reflector assemblies	64	2	8	Safety
Fuel assembly pitch (mm)	218.110	3	8	Safety
Gap between fuel assemblies (mm)	1.702	4	8	Safety
Active core length (mm)	3571.24	5	12	Regulating
Total core length (mm)	4007.42	6	8	Regulating
		7	9	Regulating
		8	8	APSR



	8	9	10	11	12	13	14	15
H	4.00 CR(7)	4.95 4Gd+BP	5.00 4Gd CR(2)	4.95 4Gd+BP	4.40 CR(7)	5.00 4Gd+BP	4.85 4Gd CR(6)	4.85 4Gd
K		4.95 4GD CR(2)	4.95 4Gd+BP	4.85 4Gd CR(4)	4.95 4Gd+BP	5.00 4Gd CR(5)	5.00 8Gd	4.95 8Gd
L			4.95 4Gd CR(6)	4.95 4Gd+BP	4.95 4Gd APSR(8)	5.00 4Gd+BP	4.40 CR(1)	4.85 4Gd
M				4.40 CR(5)	4.95 BP	4.95 4Gd CR(3)	5.00 8Gd	
N					5.00 4Gd CR(7)	5.00	4.95 4Gd+BP	
O						5.00 4Gd		
P								
R								

A C – Control rod type and group number
B B – Gd and BP pin configuration
C A – Fuel enrichment, unit: wt.%

Generation of cross section sets for Exercise I-3

- Exercise I-3
  - Standalone neutronics simulation
  - Fresh fuel
  - Hot zero power (HZP) steady-state
  - All rods inserted (ARI)

- 1000 sets of perturbed cross section
  - 56g-ENDF/B VII.1 library
  - 56g-ENDF/B v7.1 covariance data library
  - Source of uncertainty: cross sections

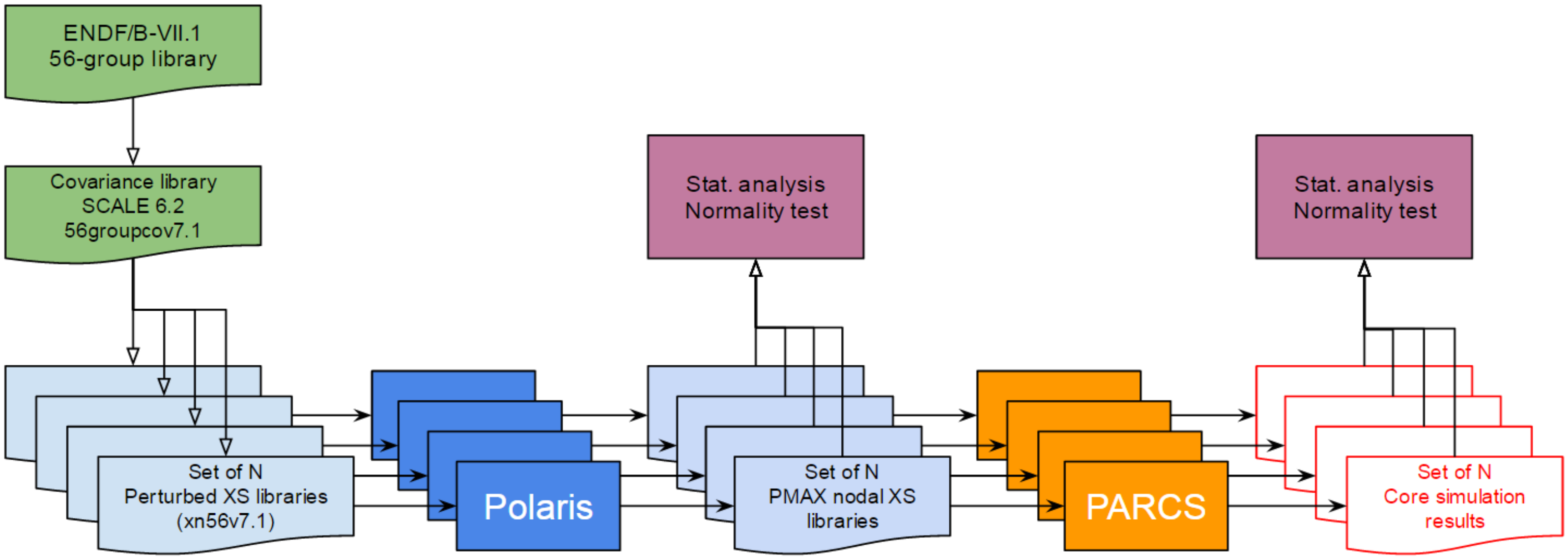
- 14 unique lattice models
  - 8 fuel lattices
  - 3 BP-loaded lattices
  - 3 reflector models

	8	9	10	11	12	13	14	15
H	4.00 CR(7)	4.95 4Gd+BP	5.00 4Gd CR(2)	4.95 4Gd+BP	4.40 CR(7)	5.00 4Gd+BP	4.85 4Gd CR(6)	4.85 4Gd
K		4.95 4GD CR(2)	4.95 4Gd+BP	4.85 4Gd CR(4)	4.95 4Gd+BP	5.00 4Gd CR(5)	5.00 8Gd	4.95 8Gd
L			4.95 4Gd CR(6)	4.95 4Gd+BP	4.95 4Gd APSR(8)	5.00 4Gd+BP	4.40 CR(1)	4.85 4Gd
M				4.40 CR(5)	4.95 BP	4.95 4Gd CR(3)	5.00 8Gd	
N					5.00 4Gd CR(7)	5.00	4.95 4Gd+BP	
O						5.00 4Gd		
P								
R								

A　C – Control rod type and group number
B　B – Gd and BP pin configuration
C　A – Fuel enrichment, unit: wt.%

Stochastic sampling using Sampler/Polaris and PARCS

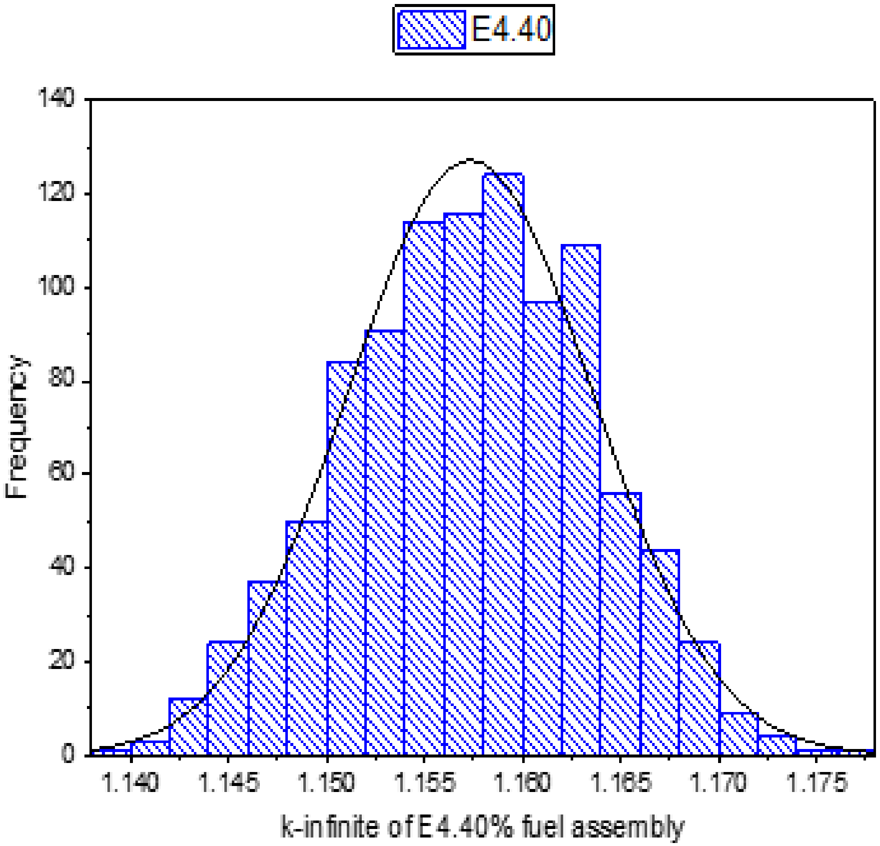
- SCALE 6.2 Sampler/Polaris
  - Sampler: General stochastic sampling method for uncertainty propagation
  - Polaris: new LWR lattice physics transport code
- GenPMAXS: Conversion of format from txtfile16 to PMAXS
- PARCS: Nodal core simulator



Exercise I-3: lattice calculation

- For all fuel assembly lattices, the uncertainty of kinf is ~0.55% or ~600 pcm for fresh fuel.

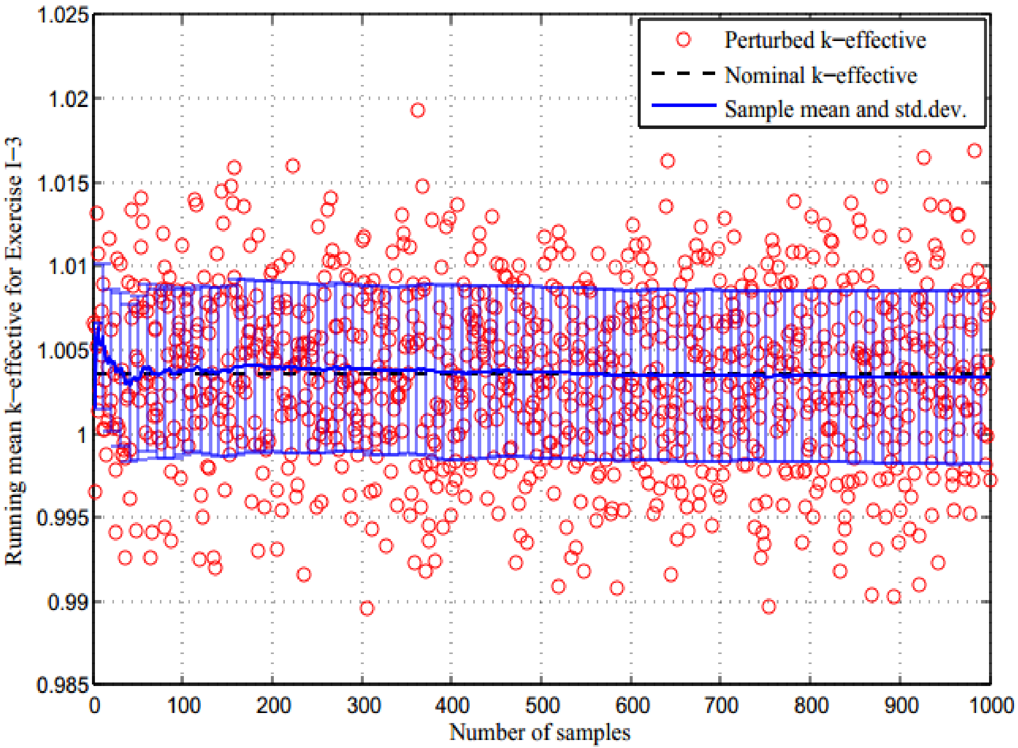
Lattice type	k_{inf} ± rel. σ
E4.00	1.12780 ± 0.55%
E4.40	1.15704 ± 0.54%
E4.85+4GD	1.15748 ± 0.54%
E4.95+BP	1.06570 ± 0.55%
E4.95+BP+4GD	1.03814 ± 0.56%
E4.95+4GD	1.16358 ± 0.53%
E4.95+8GD	1.13113 ± 0.54%
E5.00	1.19453 ± 0.53%
E5.00+BP+4GD	1.04129 ± 0.56%
E5.00+4GD	1.16657 ± 0.53%
E5.00+8GD	1.13422 ± 0.54%



Exercise I-3: running mean *k*-eff

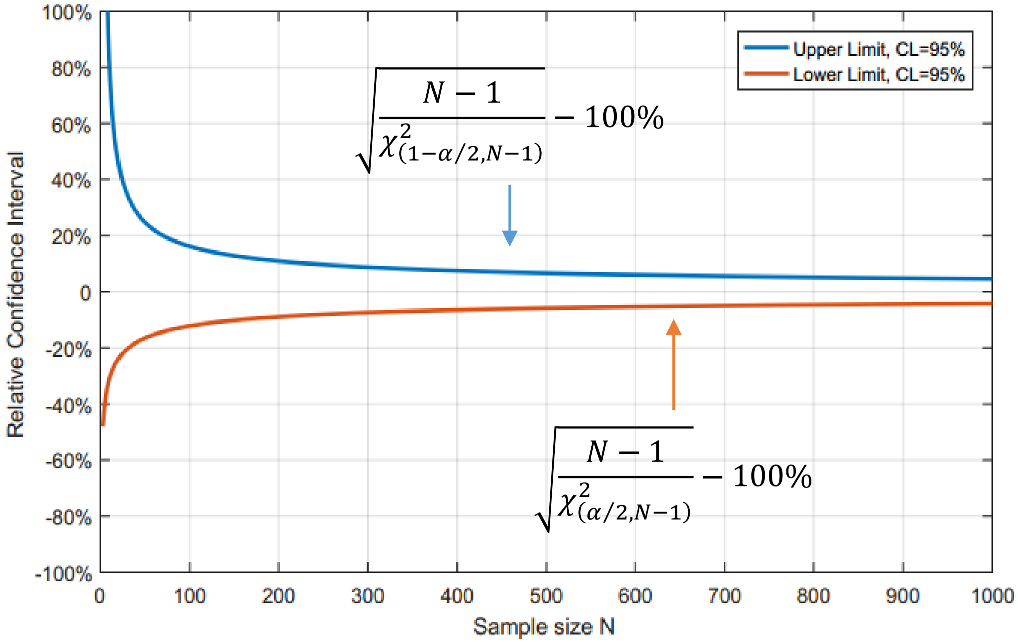
- 2-group cross sections generated for 1 nominal + 1000 samples
- Core condition: fresh, HZP, ARI
- Running mean and uncertainty do not change much when *N* > 400
- The standard deviation of *k*-eff with 1000 and 150 samples are both ~0.51%

Nominal k_{eff}	1.00361
Sample mean k_{eff} ± rel. σ (1000 samples)	1.00340 ± 0.51%
Sample mean k_{eff} ± rel. σ (150 samples)	1.00374 ± 0.51%
Diff. from nominal k_{eff}	0.01%
Diff. from mean k_{eff} of 1000 samples	0.03%



Confidence intervals for *k*-eff population standard deviation

- But a larger sample size will yield narrower confident intervals*
- A sample size of 100 yields >10% relative confidence interval
- It is not acceptable if *N* = 100 is used to investigate some effect that has < 10% impact on sample standard deviation



Evolution of 95% relative confidence intervals with sample size

Relative confidence interval for confidence level of 95%

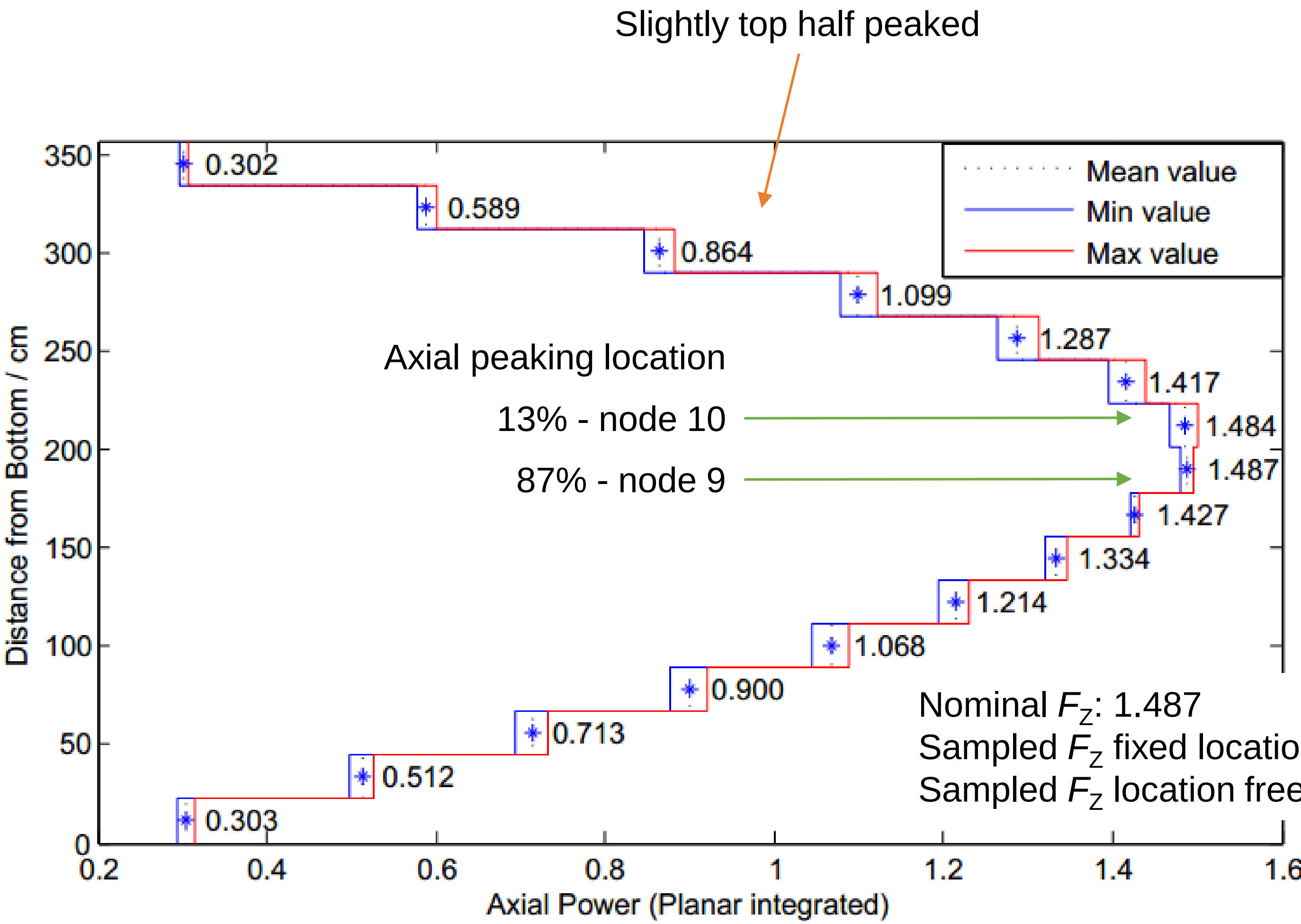
Sample size *N*	lower limit	upper limit
100	87.8%	116.2%
500	94.2%	106.6%
1000	95.8%	104.6%

How to choose sample size *N*?

- Depends on users' need
  - CL/confidence interval
  - Convergence of std
- Depends on response of interest
- Is it possible to let Sampler choose *N*?

* F. Bostelmann et al., "Some comments on the GRS MHTGR results of Phase I,", IAEA CRP on HTGR UAM: RCM-4, Vienna, May 22-25, 2017

Exercise I-3: axial power profile



Nominal F_Z: 1.487
Sampled F_Z fixed location (node 9): 1.487 ± 0.14%
Sampled F_Z location free: 1.487 ± 0.16%

Exercise I-3: radial power profile

Radial peaking factor F_R
Nominal: 1.683
Sampled: 1.683 ±0.55%

Fixed peaking location
Fuel enrichment 4.95%

Control rod locations

Large uncertainty due to:
low power,
normalization process

0.756 ±1.42%	0.698 ±1.41%	0495 ±0.99%					
0.865 ±0.46%	1.111 ±0.85%	0.730 ±0.54%	0.795 ±1.28%	0.542 ±2.01%			
1.043 ±0.62%	1.007 ±0.33%	1.211 ±0.53%	1.073 ±1.21%	1.412 ±2.72%	0.933 ±3.09%		
0.909 ±1.69%	1.202 ±0.74%	1.683 ±0.55%	1.454 ±0.87%	1.246 ±1.65%	1.412 ±2.72%	0.542 ±2.01%	
0.964 ±2.58%	0.945 ±2.06%	1.266 ±0.80%	1.184 ±0.27%	1.454 ±0.87%	1.073 ±1.21%	0.795 ±1.28%	
0.768 ±3.86%	0.896s ±3.30%	0.926 ±2.38%	1.266 ±0.80%	1.683 ±0.55%	1.211 ±0.53%	0.730 ±0.54%	0.495 ±0.99%
0.752 ±4.72%	0.714 ±4.43%	0.896 ±3.30%	0.945 ±2.06%	1.202 ±0.74%	1.007 +±0.33%	1.111 ±0.85%	0.698 ±1.41%
0.589 ±5.34%	0.752 ±4.72%	0.768 ±3.86%	0.964 ±2.58%	0.909 ±1.69%	1.043 ±0.62%	0.865 ±0.46%	0.756 ±1.42%

Ex III-1: core condition and exposure map available

- Currently only focusing on steady state neutronics calculation
- HFP condition
  - Reactor power = 100% rated power (2771.9 MW);
  - Average fuel temperature = 921 K, inlet moderator temperature = 562.67 K, outlet moderator temperature = 592.7 K;
  - Control rod groups 1–6 completely withdrawn, group 7 completely inserted and group 8 (APSR) 53.8% inserted;
  - Core inlet pressure = 15.36 MPa;
  - Core flow rate = 16546.04 kg/s.

- HZP condition
  - Fuel temperature = 551 K, moderator temperature = 551 K and moderator density = 766 kg/m^3;
  - Control rod groups 1–4 completely withdrawn, groups 5–7 completely inserted and group 8 (APSR) 70% inserted.

	8	9	10	11	12	13	14	15
H	1 52.863	2 30.192	3 56.246	4 30.852	5 49.532	6 28.115	7 53.861	8 55.787
K		9 57.945	10 30.798	11 55.427	12 29.834	13 53.954	14 25.555	15 49.166
L			16 57.569	17 30.218	18 54.398	19 27.862	20 23.297	21 47.300
M				22 49.712	23 28.848	24 52.846	25 40.937	
N					26 48.746	27 23.857	28 41.453	
O						29 37.343	A B	
P								

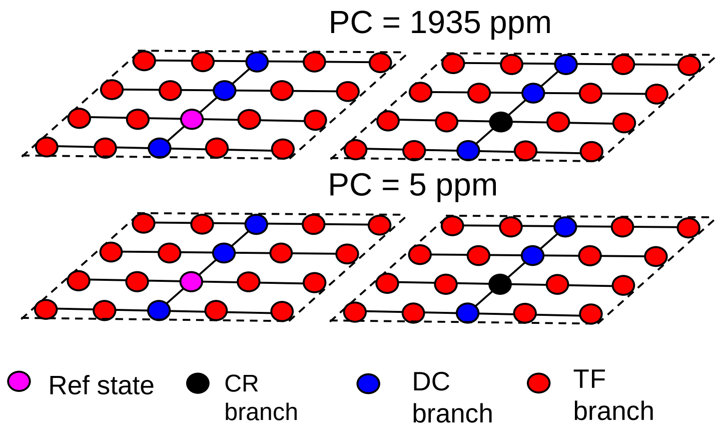
EOC assembly burnup map

Parameterized cross section generation: range of state variables

- Same approach as in Ex I-3: Polaris/Sampler
- State variables: fuel temperature, coolant density, and control rod insertion.
- Boron concentration fixed at 1935 ppm and 5 ppm for BOC and EOC, respectively.

State variables	State points calculated
Fuel temperature (K)	551, 921, 1780, 2400, 3000
Boron Concentration (ppm)	5, 1935
Coolant density (g/cc)	0.660, 0.702, 0.733, 0.770
Control rod insertion	Yes, no
APSR insertion	Yes, no

For non-APSR assemblies: 5×4×2=40 state points for both BOC and EOC state



For APSR lattice: 5×4×4=80 state points for both BOC and EOC state, respectively.

Exercise III-1: keff , uncertainties, and normality tests

State	Nominal k_{eff}	Sample mean k_{eff} ± rel. σ	Anderson-Darling normality test
BOC HZP	1.01979	1.01986 ± 0.44%	Pass
EOC HZP	1.04263	1.04276 ± 0.45%	Pass
BOC HFP	1.01125	1.01136 ± 0.46%	Pass
EOC HFP	1.02885	1.02902 ± 0.47%	Pass

- The 150 core keff's could be regarded as normally distributed.
- The uncertainties for keff is 0.44-0.47%.
- They are smaller than the uncertainty of Exercise I-3 fresh core keff (0.51%), because there are more heavy mental in fresh core and only the perturbation in cross section is taken into account at this stage.

- For N = 150, rel. confidence interval for CL of 95% is [-10.18%, 12.80%]

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Exercise III-1: axial power profile at HFP state

HFP BOC

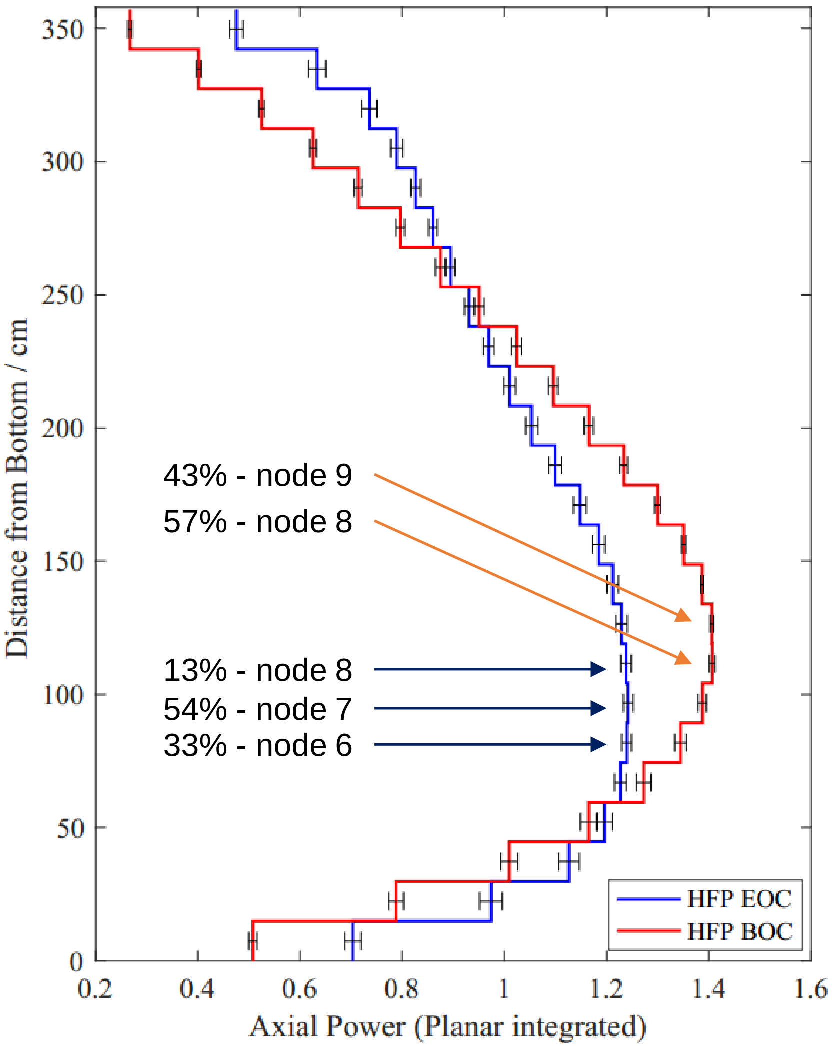
Nominal F_z: 1.406
150 sample mean F_z location free: 1.408 ± 0.33%
150 sample mean F_z location fix (node 8): 1.406 ± 0.23%

HFP EOC

Nominal F_z: 1.242
150 sample mean F_z location free: 1.243 ± 0.75%
150 sample mean F_z location fix (node 7): 1.242 ± 0.77%

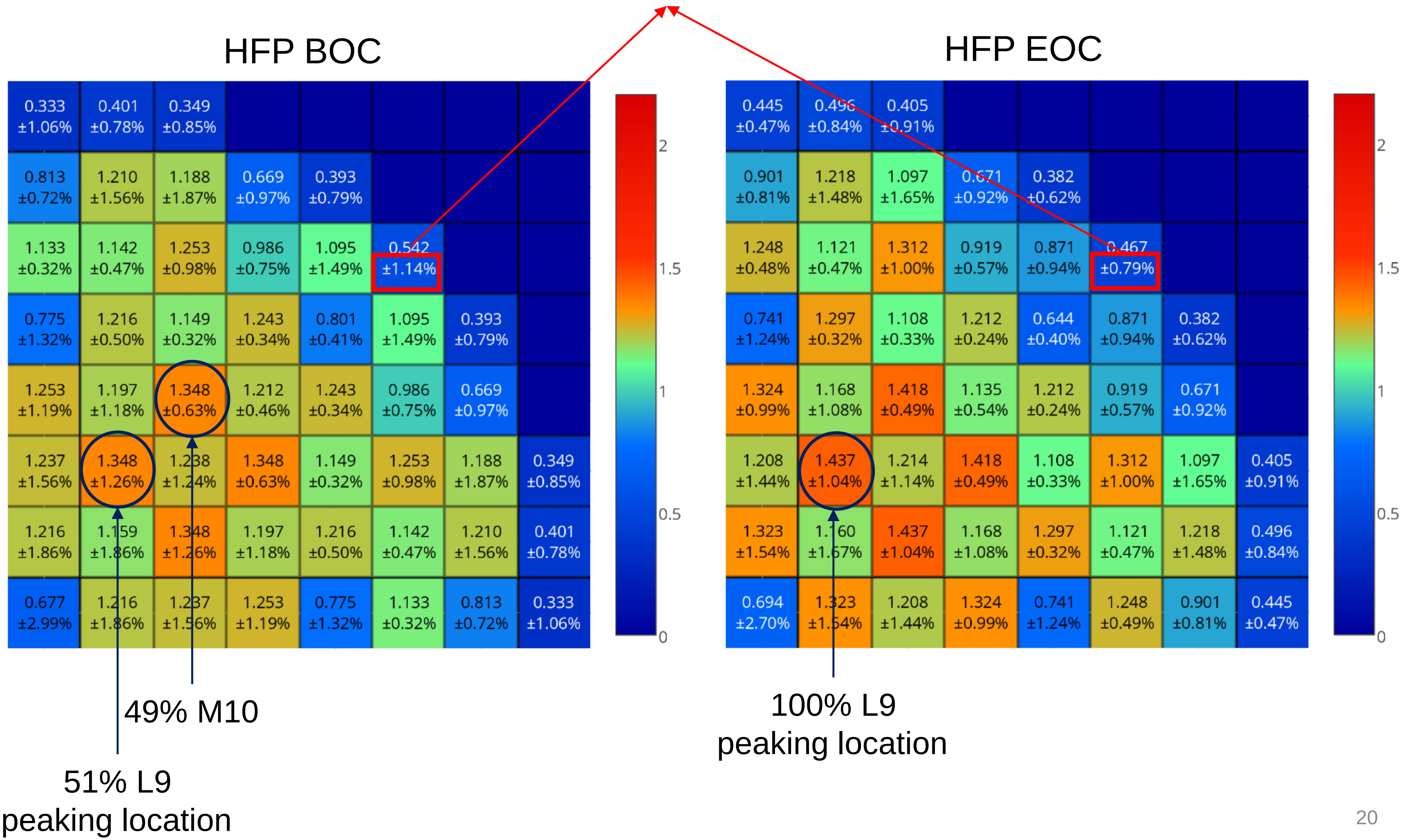
Axial powers peak in bottom half core:
Smaller moderator temperature
→ larger moderator density.

Axial power profile is flattened towards EOC.

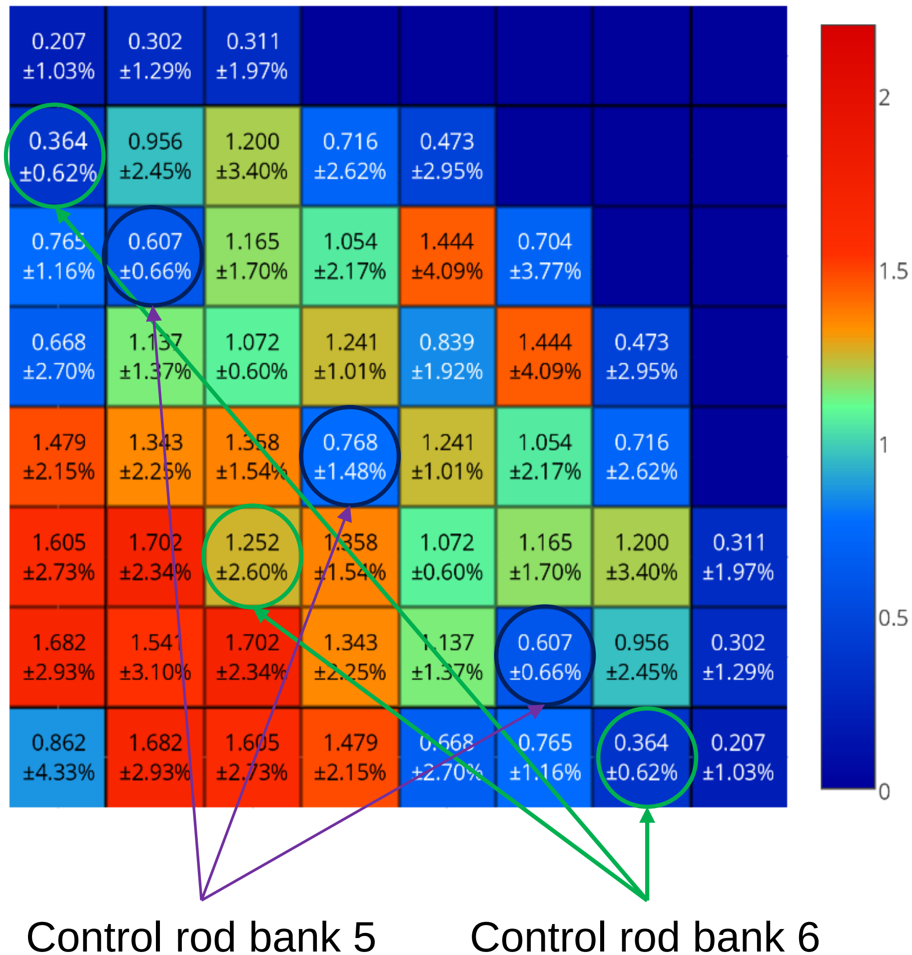


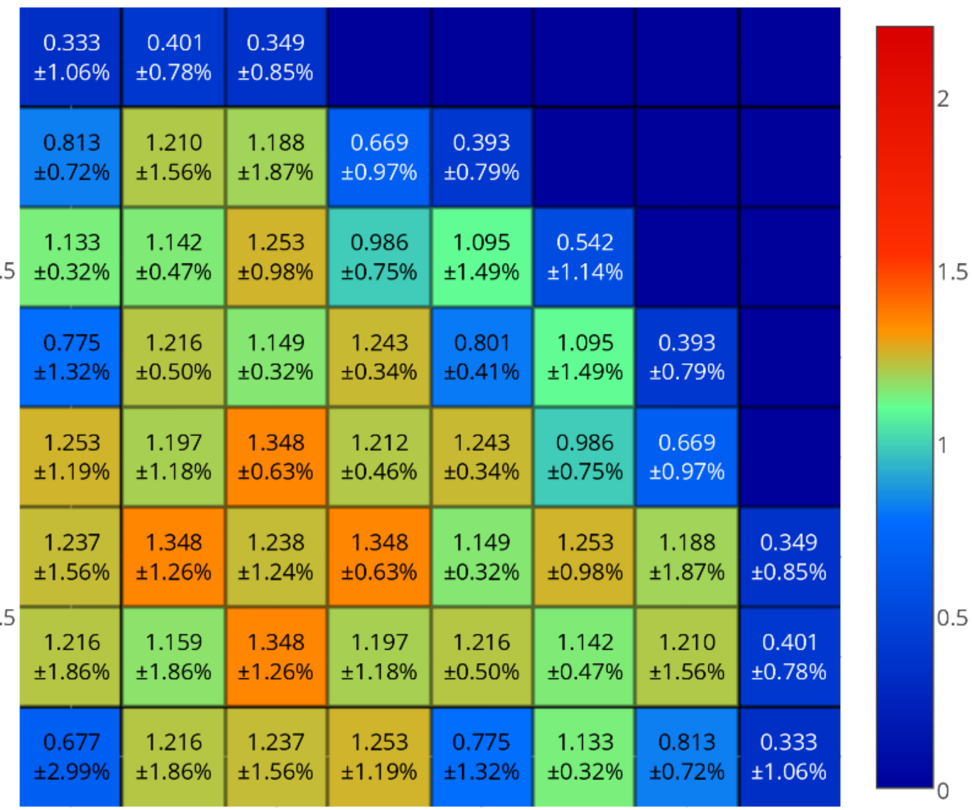
Exercise III-1: radial power distribution at HFP

Uncertainty smaller at EOC due to flattened flux distribution



Exercise III-1: radial power distribution at BOC





Summary on LWR UAM activities

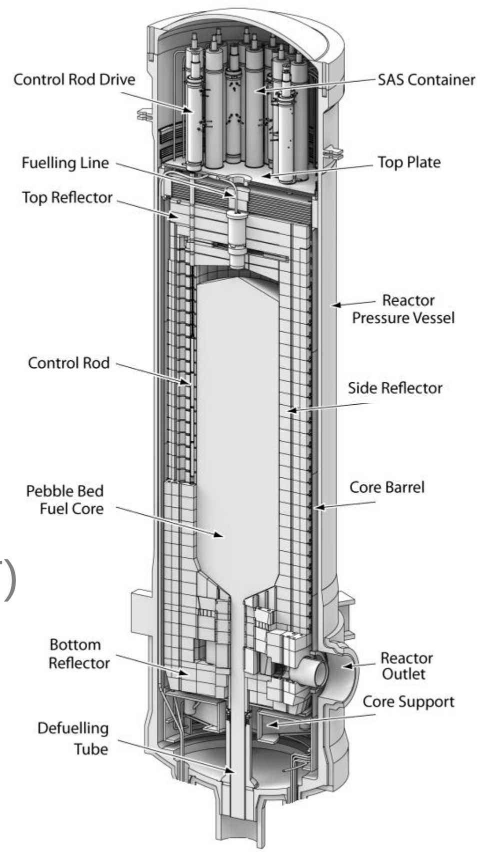
- Cross section sets prepared for TMI-1 case in NEMTAB and PMAX format using Polaris/Sampler in SCALE 6.2.1
- Preliminary results obtained for TMI-1 steady-state simulations using statistical sampling method
  - Core k_{eff}, axial power peaking factor and radial power peaking factor are analyzed with associated uncertainties
  - Anderson-Darling normality test performed
- Ongoing work
  - It was reported that pin-by-pin calculation yields a non-normal power peaking factors. In contrast, the nodal solution of the power peaking factors are normally distributed.
  - Continue with depletion and transient (REA) simulations

Capability needed
- Shape function generated by Polaris
- Now available in NEWT output

IAEA CRP on HTGR UAM: PBR-250

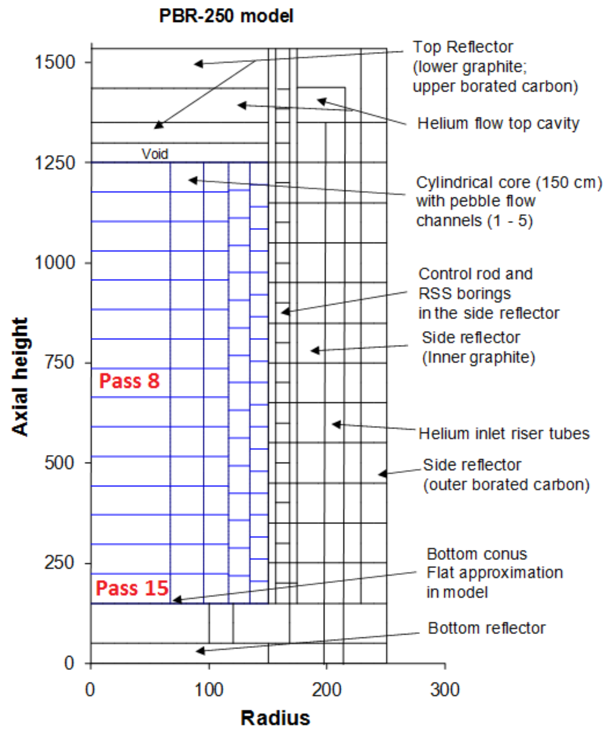
Lidong Wang, Fu Li
Institute of Nuclear and New Energy Technology (INET)
Tsinghua University, China

Jason Hou, Kostadin Ivanov
Department of Nuclear Engineering
North Carolina State University



High Temperature Gas-cooled Reactor (HTGR) Uncertainty Analysis in Modeling (UAM) was initiated in 2012

- Core configurations
  - Prismatic
  - Pebble bed: representative 250 MWth Pebble Bed Reactor design (PBR-250)
- Objectives (following ideas of NEA/OECD UAM on LWRs)
  - To subdivide system into steps
  - To identify inputs, outputs and propagated uncertainties for each step
  - To calculate resulting uncertainty in each step
  - To propagate the results in integral system
- Peculiarities of HTGR
  - Fuel design - TRISO
  - Large graphite quantity
  - High temperature
- In the current study, focuses have been placed on
  - Exercise I-1 and I-2
  - HTGR modeling options
  - Nuclear data uncertainty



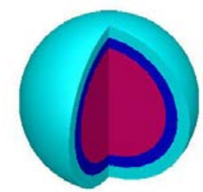
SCALE modules used in this study

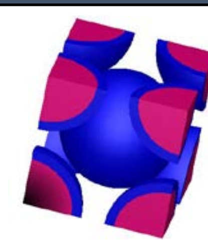
- SCALE versions
  - 6.1, 6.2, 6.2.2
- SCALE modules
  - KENO-VI, TSUNAMI-3D
- SCALE libraries
  - Nuclear data libraries: ENDF/B VII.0, ENDF/B VII.1
  - Covariance libraries: 44groupcov, 56groupcov7.1

Benchmark Phase I: local standalone neutronics simulation

- Exercise I-1
  - single pebble or “cell” calculation
- Model parameters
  - 7g heavy metal per pebble
  - White/reflective boundary

- Exercise I-2
  - core unit or “assembly” calculation
- Packing structure
  - BCC / HCP / “Dummy” Pebble

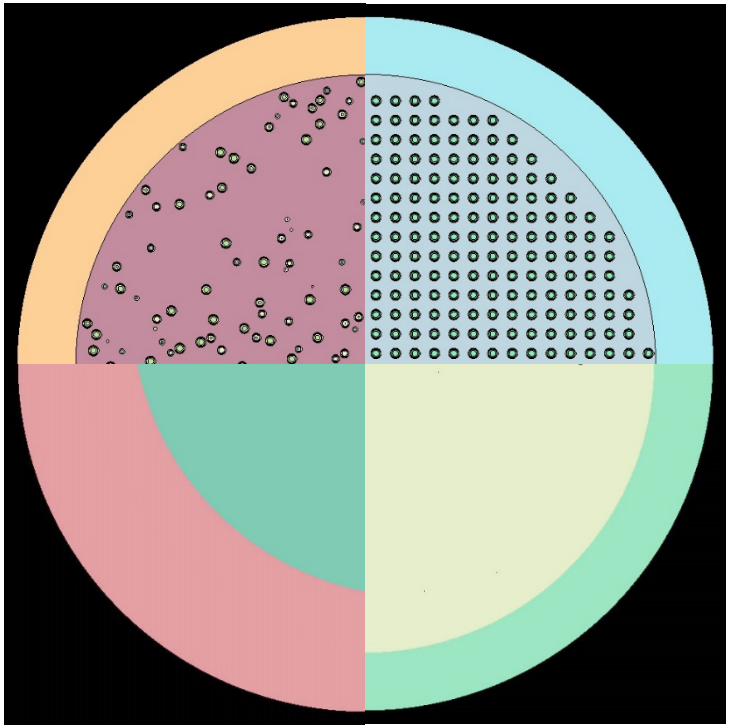
Exercise	Sub-cases	State	Enrichment	Geometry
Exercise I-1	a: Fresh fuel	CZP (cold zero power, 293K)	8.9% (4.2%*)	
	b: Batch 113 burned fuel[†]	HFP (hot full power, 900K)	--	

Exercise	Central	Case neighbors	State	Geometry
Exercise I-2	Batch 113	a: Batch 113 b: Batch 225 c: Fresh fuel d: Graphite	CZP	
			HFP	

[*] 4.2% is the fuel enrichment usually used in HTGR criticality in fresh core
[†] Burn-up of this representative fuel sphere is ~63,000 MWd/T

Exercise I-1: single pebble

- Modeling approaches (Ex I-1a only)
  - Various levels of geometry simplification
  - Effect on multiplication factor
- Effect of ND library (Ex I-1a, CZP & HFP state)
- Uncertainty quantification



- Modeling with KENO-VI
  - Explicit model of coated particles (lattice)
  - Homogenized fuel region with
  - DOUBLEHET unit cell
  - Homogenized fuel region with RPT
- Modeling with Serpent-2
  - Randomly distributed particles
  - Code-to-code verification

Effect of modeling approaches on multiplication factors

- Ex I-1a, ENDF/B VII.1

	Case	CZP (293K)		HFP (900K)	
		$k_{eff} \pm \sigma$	Δ[pcm]	$k_{eff} \pm \sigma$	Δ[pcm]
With double heterogeneity treatment	KENO-VI CE Lattice	1.57841±0.00019	reference	1.50277±0.00014	reference
	Serpent-2 Lattice	1.57883±0.00010	42	1.50298±0.00010	21
	Serpent-2 Random	1.57656±0.00010	-185	1.50071±0.00010	-206
	KENO-VI MG DH	1.57535±0.00015	-306	1.49904±0.00014	-373
Approximate homogenization	Serpent-2 HM	1.46188±0.00008	**-11,653**	1.37548±0.00010	**-12,729**
	KENO-VI CE HM	1.46131±0.00014	-57	1.37559±0.00015	11
	KENO-VI MG HM	1.45914±0.00021	-274	1.37378±0.00025	-170

- CE Monte Carlo methods produce consistent results using lattice model: Δ*k* < 50 pcm
- Results associated with random distribution of particles are in between those of lattice and DH models
- CE Lattice model vs. MG DOUBLEHET model: -306 & -373 pcm

Effect of nuclear data libraries (Ex I-1a, 8.9% enrichment)

- Multiplication factor

Case	CZP(293K)			HFP(900K)		
	ENDF/B VII.0	ENDF/B VII.1	Δ[pcm]	ENDF/B VII.0	ENDF/B VII.1	Δ[pcm]
KENO-VI CE Lattice	1.58613±0.00019	1.57841±0.00019	772	1.50948±0.00013	1.50277±0.00014	671
Serpent-2 Lattice	1.58580±0.00010	1.57883±0.00010	697	1.50932±0.00010	1.50298±0.00010	634
Serpent-2 Random	1.58379±0.00010	1.57656±0.00010	723	1.50717±0.00010	1.50071±0.00010	646
KENO-VI MG DH	1.58309±0.00016	1.57535±0.00015	774	1.50694±0.00013	1.49904±0.00014	790
Serpent-2 HM	1.46737±0.00008	1.46188±0.00008	549	1.38110±0.00010	1.37548±0.00010	562
KENO-VI CE HM	1.46763±0.00015	1.46131±0.00014	632	1.38176±0.00016	1.37559±0.00015	617
KENO-VI MG HM	1.46589±0.00021	1.45914±0.00021	675	1.37954±0.00020	1.37378±0.00025	576

- 500-800 pcm difference was found when comparing the results of ENDF/B VII.0 and ENDF/B VII.1 for all models at both CZP and HFP states.

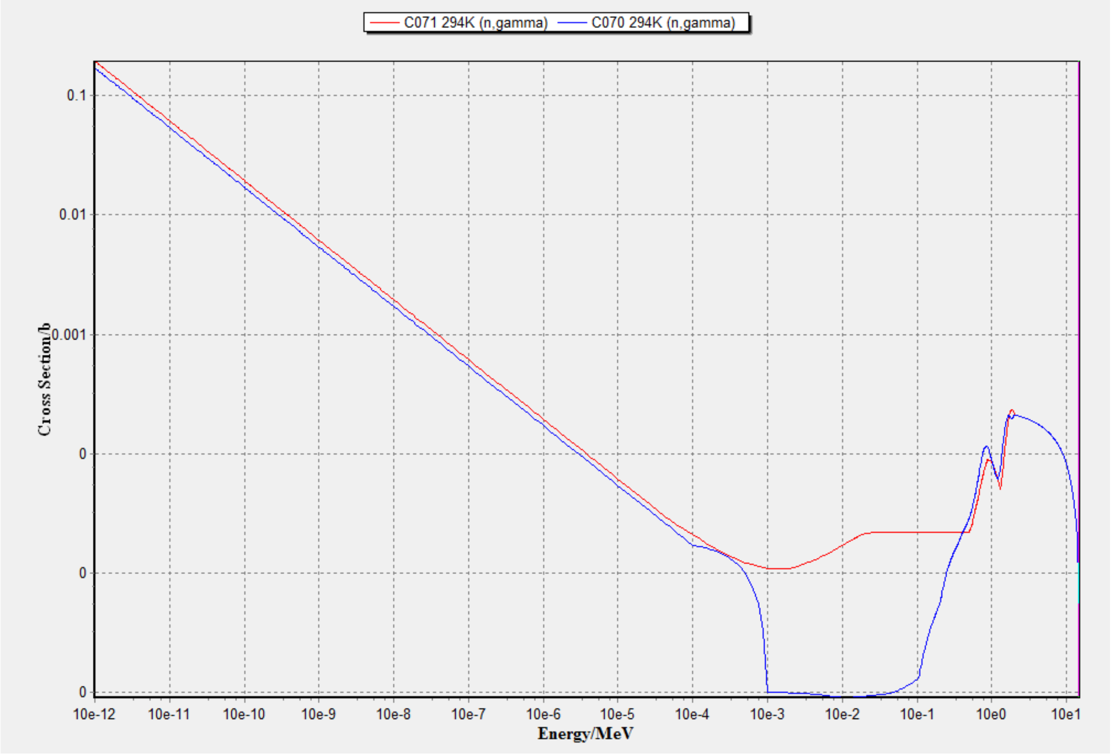
Nuclear data difference: carbon (n,gamma) reaction

- Relatively large difference between ENDF/B-VII.0 and -VII.1
- Effect on criticality calculation

for a coated particle ~200 pcm

for a single pebble ~700 pcm

for a core unit ~1100 pcm



Uncertainty quantification (UQ) following sensitivity based approach

- Various options in TSUNAMI-3D were tested
  - MG: the doubly heterogeneous effect cannot be ignored
  - CE-IFP*: huge memory footprint
  - CE-CLUTCH†: mesh grid with enough neutron histories is required
    - Convergence of importance function $F^*(r)$ should be guaranteed
    - Choice of mesh size and neutron history in each mesh is important but heavily relies on user's experience
    - Sensitivity coefficients obtained from TSUNAMI-3D should always be verified with direct perturbation method (DPM) results.
- Calculations performed for the following
  - MG/CE TSUNAMI-3D (Ex I-1a)
  - CE TSUNAMI-3D (Ex I-1b)
  - Parametric study for CE-CLUTCH
  - Influence of temperature
  - Influence of covariance libraries

* Iterated Fission Probability

† Contribution-linked Eigenvalue Sensitivity/Uncertainty Estimation via Tracklength Importance Characterization

MG/CE TSUNAMI-3D calculations (SCALE6.2, Ex I-1a)

- Related issues
  - COV-Lib couldn't be switched to 44groupcov in CE TSUNAMI-3D sequence – resolved in SCALE 6.2.2
  - MG mode with Doublehet option succeed, which was unexpected
- Ex I-1a (fresh fuel) CZP state results

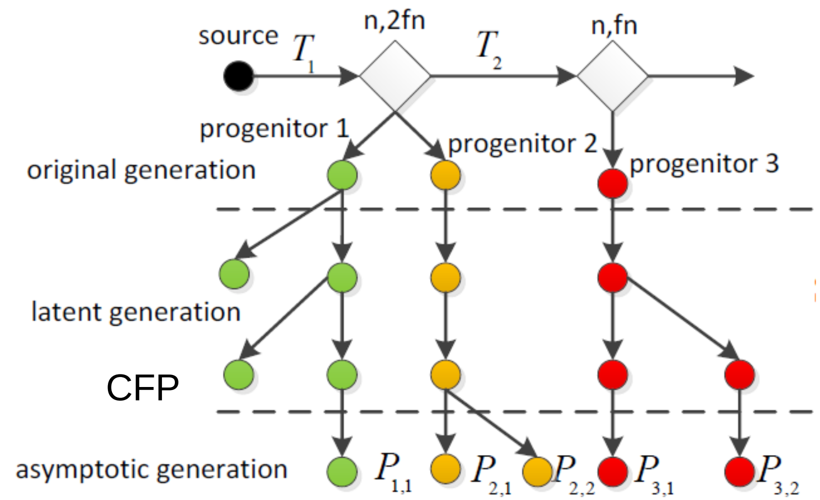
TSUNAMI	ND_Lib	COV_Lib	keff	Uncertainty (%k/k)
MG	ENDF/B VII.0	44groupcov	1.58309±0.00016	0.455390±0.000040
		56groupcov7.1	1.58309±0.00016	0.497242±0.000016
CE-IFP		56groupcov7.1	1.58553±0.00039	0.500800±0.000430
CE-CLUTCH		56groupcov7.1	1.58580±0.00022	0.500440±0.000380
MG	ENDF/B VII.1	44groupcov	1.57586±0.00015	0.454402±0.000040
		56groupcov7.1	1.57586±0.00015	0.493352±0.000020
CE-IFP		56groupcov7.1	1.57970±0.00040	0.503500±0.000480
CE-CLUTCH		56groupcov7.1	1.57975±0.00014	0.502950±0.000250

MG TSUNAMI-3D UQ results are smaller than CE TSUNAMI-3D UQ results, as the implicit effect is ignored.

Should always use consistent ND and COV libraries: ENDF/B-VII.0+44groupconv; ENDF/B-VII.0+56groupconv7.1

Ex I-1b: Batch-113 burned Fuel (CZP state)

- IFP CE TSUNAMI-3D
  - ~40G memory for CFP (number of latent generation) = 1
  - CFP usually is 5-10
  - Compared with ~9G for fresh fuel (4 isotopes)
  - Not applicable to larger geometry
- CLUTCH CE TSUNAMI-3D



IFP Scheme

TSUNAMI	Lib	Temp	Uncertainty (%k/k)
IFP	ENDF/B VII.1 56groupcov	293	0.52038±0.00043
CLUTCH			0.51575±0.00039
IFP		900	0.51256±0.00044
CLUTCH			0.51834±0.00029

Influence of temperature on uncertainties

- IFP results were collected in test calculations that didn't follow recommended setup

Exercise	TSUNAMI	Lib	Temp	*k*-eff	Uncertainty (%k/k)
Ex I-1a	IFP	ENDF/B VII.1 56groupcov	293K	1.57965±0.00029	0.50130±0.00032
			900K	1.50402±0.00030	0.51565±0.00038
	CLUTCH		293K	1.57975±0.00014	0.50295±0.00025
			900K	1.50337±0.00014	0.51834±0.00029
Ex I-1b	IFP		293K	1.09173±0.00015	0.51575±0.00039
			900K	1.05889±0.00043	0.51472±0.00064
	CLUTCH		293K	1.09193±0.00020	0.52038±0.00043
			900K	1.05908±0.00016	0.51258±0.00044

Sensitivity analysis is required to understand the decrease of rel. uncertainty with temperature for burned fuel.

Influence of libraries / covariance (CLUTCH)

- CE TSUNAMI-3D IFP requires large memory
- Only CE TSUNAMI-3D CLUTCH results are available

Exercise	Mat.	Temp. (K)	Lib / Cov	keff	Uncertainty (%k/k)
Ex I-1a	8.9%	293	7.1 / 56	1.57975±0.00014	0.50295±0.00025
			7.0 / 44	1.58689±0.00013	0.45096±0.00031
		900	7.1 / 56	1.50337±0.00014	0.51834±0.00029
			7.0 / 44	1.50980±0.00015	0.47267±0.00038
	4.2%	293	7.1 / 56	1.42819±0.00012	0.55577±0.00033
			7.0 / 44	1.43954±0.00014	0.51578±0.00047
		900	7.1 / 56	1.34920±0.00014	0.57858±0.00039
			7.0 / 44	1.36010±0.00013	0.52876±0.00054
Ex I-1b	Batch 113	293	7.1 / 56	1.09193±0.00020	0.52038±0.00043
			7.0 / 44	1.09700±0.00016	0.55383±0.00050
		900	7.1 / 56	1.05908±0.00016	0.51258±0.00044
			7.0 / 44	1.06354±0.00015	0.60715±0.00046

- Impact of nuclear data library
- Spectral effect
- Impact of composition

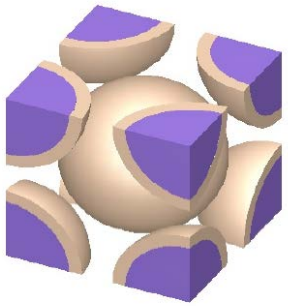
Top 7 Contributors to k_{eff} Uncertainty

- Impact of fuel enrichment
- Results obtained for ENDF/B-VII.1 + 56g cov
- Spectral shift affects contribution to *k*-eff uncertainty

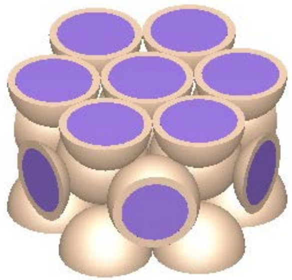
No.	8.9%wt		4.2%wt	
	Matrix	Contribution	Matrix	Contribution
1	U-235 $\bar{\nu}$	3.7866E-01	U-235 $\bar{\nu}$	3.8136E-01
2	U-235 (n,γ)	2.0919E-01	U-238 (n,γ)	2.2987E-01
3	U-238 (n,γ)	1.6196E-01	U-235 (n,γ)	1.9664E-01
4	U-235 $(n,f)(n,\gamma)$	1.0949E-01	Graphite (n,γ)	1.7274E-01
5	Graphite (n,γ)	9.0193E-02	U-235 $(n,f)(n,\gamma)$	1.2147E-01
6	Grphite (n,n)	8.2684E-02	U-235 (n,f)	9.3696E-02
7	U-235 (n,f)	7.1330E-02	Grphite (n,n)	7.6731E-02

Exercise I-2: core unit or "assembly" calculation

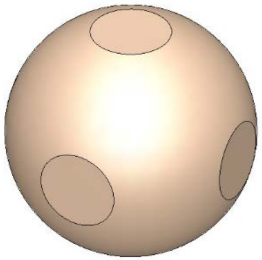
- Packing study: BCC, HCP, "Dummy" Pebble
- BCC sub-cases
  - Central fuel sphere: Batch 113
  - Neighbors
    - a-Batch 113; b-Batch 225; c-Fresh fuel d-Graphite
  - CZP-293k; HFP-900K
- Three geometries with same pack fraction (61%)
  - BCC structure
    - Cubic boundary, reflective/periodic BC
    - 2 pebbles in total
  - HCP structure
    - Hexagonal prismatic boundary, periodic BC
    - 13 spheres in total
  - Dummy pebble
    - Outer radius is enlarged (3 cm to 3.013 cm)
    - But enclosed by the cubic boundary
    - to satisfy 61% packing fraction



BCC



HCP



Dummy pebble

Criticality calculation and UQ results

- Multiplication factor ENDF/B VII.1, CZP, all 4.2% enrichment
  - Impact of geometry is negligible as long as the pack fraction is maintained

Model	BCC	HCP	Dummy pebble
KENO-VI CE Lattice	1.42787±0.00014	1.42811±0.00015	1.42835±0.00014
Serpent-2 Lattice	1.42789±0.00008	1.42810±0.00008	1.42817±0.00008
Serpent-2 Random	1.42639±0.00008	1.42641±0.00008	1.42681±0.00008
KENO-VI MG DH	1.42547±0.00011	1.42540±0.00012	1.42560±0.00011

- UQ using TSUNAMI-3D CLUTCH for BCC sub-cases
  - Central pebble is batch 113 burned fuel sphere

Sub-cases	CZP		HFP	
	keff	Uncertainty %	keff	Uncertainty %
a: batch 113	1.09163±0.00015	0.48780±0.00032	1.05913±0.00014	0.50412±0.00041
b: batch 225	0.99503±0.00016	0.54570±0.00050	0.98523±0.00014	0.54084±0.00045
c: fresh fuel	1.35637±0.00017	0.48444±0.00027	1.28407±0.00014	0.48116±0.00032
d: graphite	1.16663±0.00015	0.54910±0.00035	1.16906±0.00015	0.51635±0.00042

Absolute uncertainties are similar

Absolute uncertainties larger due to graphite contribution

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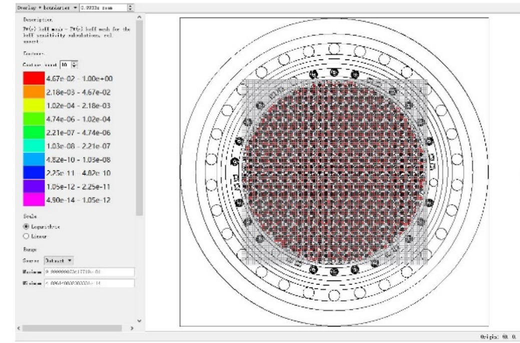
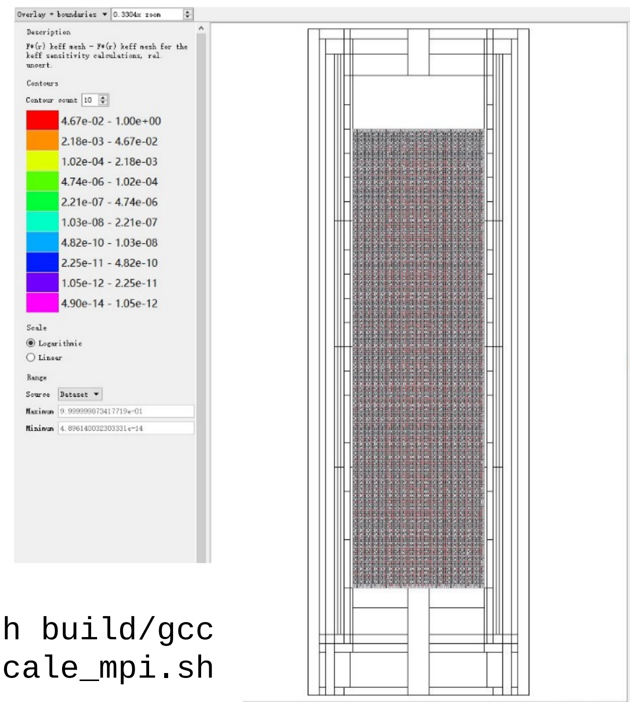
Summary on HTGR CRP activities

- Exercise I-1 single pebble
  - Study on modeling approaches (only for Ex I-1a)
    - Various levels of geometry simplification
    - Effect on multiplication factor (CZP & HFP state)
  - Effect of ND and COV library (CZP & HFP state)
  - Uncertainty quantification
- Exercise I-2 core unit
  - Packing study
  - Uncertainty quantification
- Ongoing work
  - PBR-250 whole-core model
  - UQ using CE TSUNAMI-3D CLUTCH →
  - Not possible without MPI support





Detailed instruction for compiling SCALE with MPI support is needed

Parallel SCALE (with MPI support)

```
cp script/configure_scale_mpi.sh build/gcc
chmod u+x build/gcc/configure_scale_mpi.sh
./configure_scale_mpi.sh ../..
```

Summary

- NCSU is performing studies on a number of Uncertainty Analysis in Modeling (UAM) benchmarks
  - NEA/OECD Light Water Reactor (LWR) UAM
  - IAEA CRP High Temperature Gas-cooled Reactor (HTGR) UAM
  - NEA/OECD Sodium-cooled Fast Reactor (LWR) UAM

- SCALE package is one of the major computational tools adapted for the benchmark specification and calculations
  - Neutronics modeling
  - Sensitivity and uncertainty (S/U) analysis
  - SCALE 6.2/6.2.1/6.2.2
  - TSUNAMI, Polaris, Sampler, KENO, etc.