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INL/CON-25-85895 Rev:0

Updates to the HTR-PROTEUS HALEU Benchmark Using Modern Analysis Methodologies

First Reactor Graphite (ReGra) Workshop

Brookhaven National Laboratory, July 8-9, 2025

DOE/NRC Criticality Safety for Commercial-Scale HALEU for Fuel Cycle and Transportation

Idaho National Laboratory

HTR-PROTEUS Benchmark Improvement Effort

Consolidation

CRIT portions of 4 IRPhEPs into 1 ICSBEP report IEU-COMP-THERM-TBD

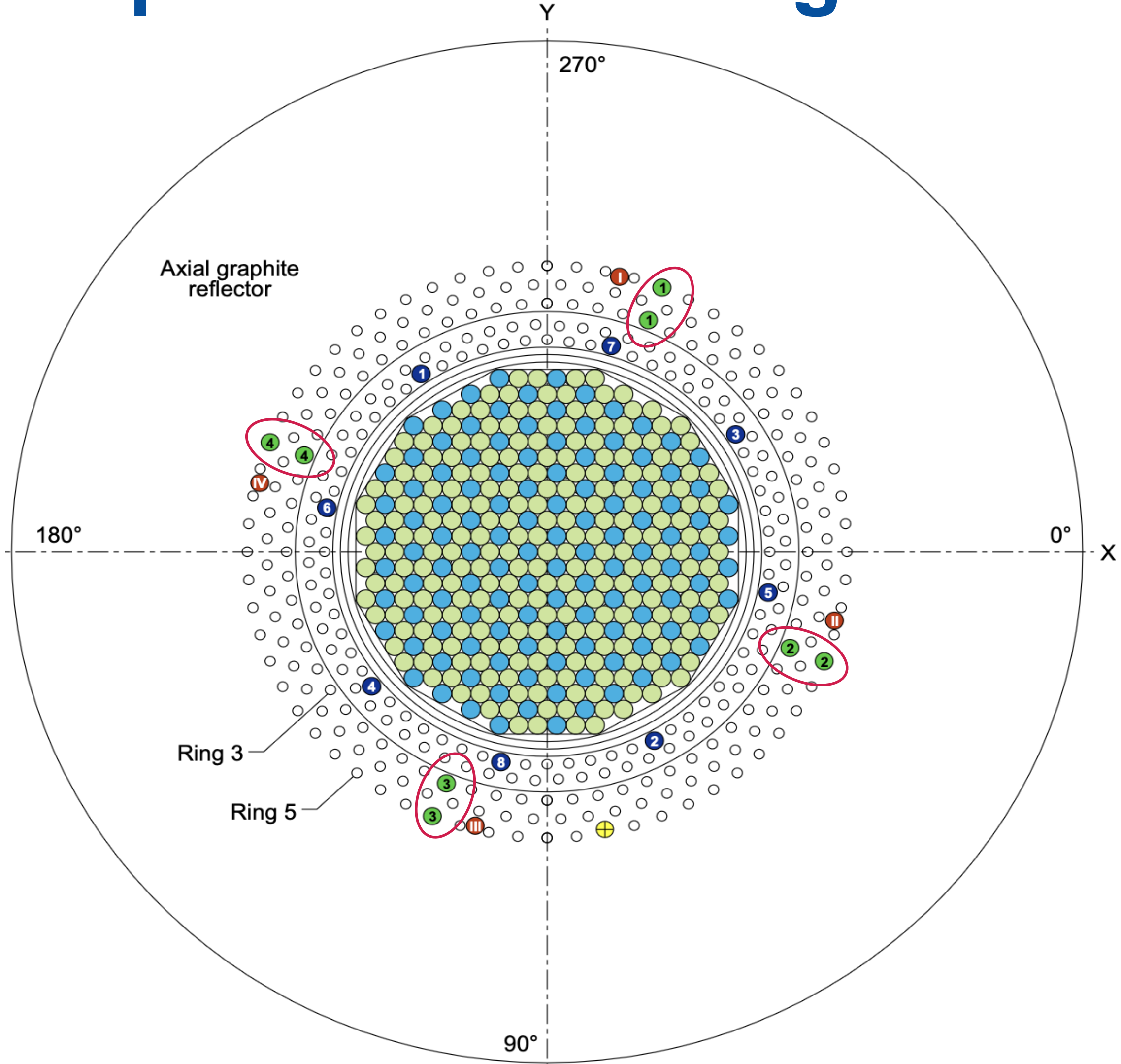
Improvements

- quality of uncertainty evaluation
- better address uncertainties in mass, density, and composition w. modern M&S tools
- adjoint sensitivity analysis via ksen card MCNP
- reduced statistical uncertainties
- better address uncertainties in random TRISO and pebble placement

Investigation

- solutions from deterministic tools
- impact of newer nuclear data libraries and TSLs
- identify, and if possible, evaluate, subcritical measurement data

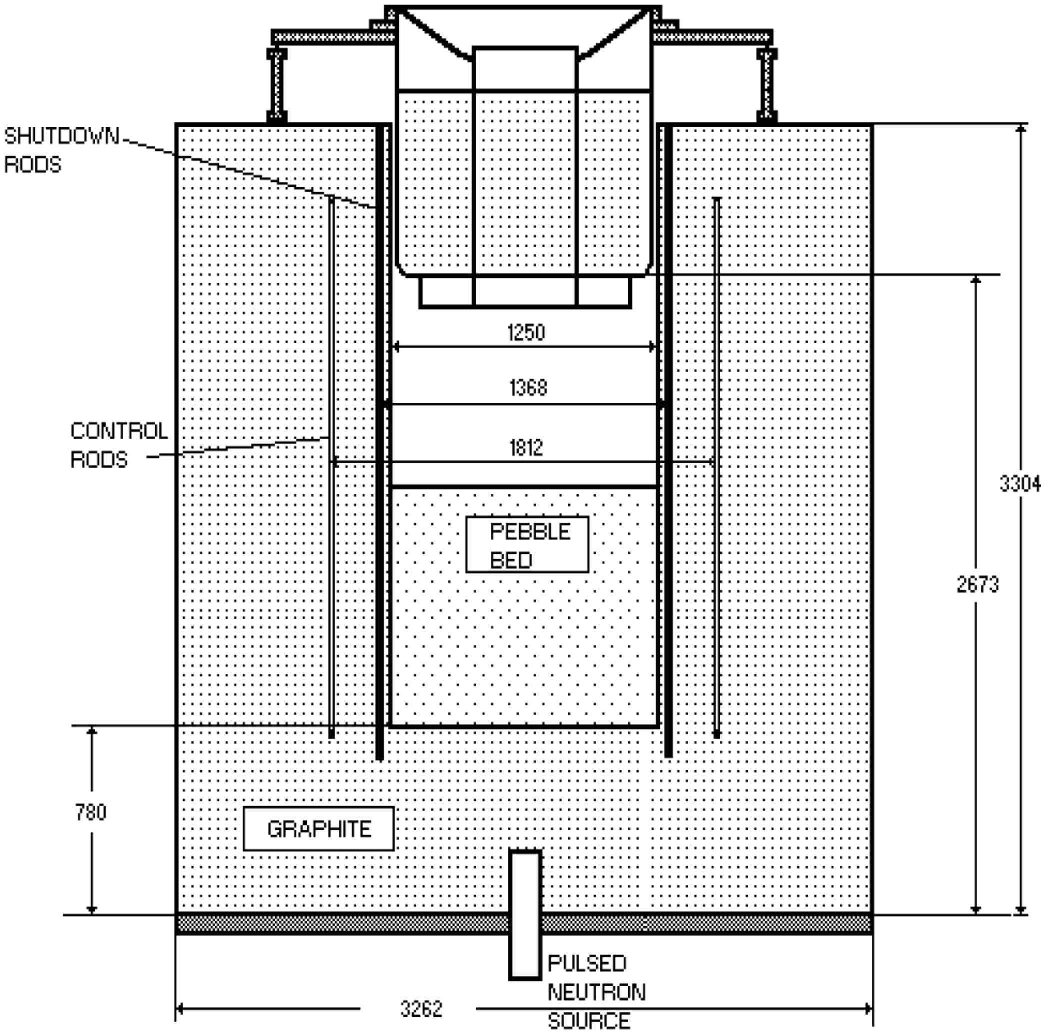
Experimental Configuration



1 - 8 Safety and shutdown rods
I - IV ZEBRA control rods
1 - 4 Withdrawable control rods (2 possible positions)
Autorod

Removable graphite rod
Fuel pebble
Moderator pebble

11-GA50002-18



Core Configurations (Revising Core 4 → 4.2 & 4.3)

Case	Core	State	Notes
1	1	1	HCP Core with ZEBRA control rods.
—	1A	*1*	*Equivalent to Core 1, ZEBRA control rods replaced with withdrawable control rods.*
2		2	Equivalent to State 1 but with graphite filler rods placed in the ZEBRA position holes.
3	2	1	Similar to Core 1A with decreased core height and increased upper graphite reflection. Used to investigate "cavity effect".
4	3	1	Similar to Core 1A with polyethylene rods added to simulate water ingress. Every available vertical channel between pebbles contained an 8.9–mm-diameter polyethylene rod.
—	*4.1*	*1*	*Random pebble loading rejected by experimenters.*
—	*4*	—	*Average core model used to evaluate uncertainties in 4.2 and 4.3 (Prior IRPhEP benchmark).*
5	4.2	1	Random pebble loading using a single pebble delivery tube.
6	4.3	1	Random pebble loading using a single pebble delivery tube (core reload for reproducibility).
—	5	*1*	*CHPOP core with coolant channels in bottom reflector open.*
7		2	Equivalent to Core 5, State #1, with coolant channels in bottom reflector filled with graphite.
—		*3*	*Reproducibility measurement*
8	6	1	Similar to Core 5 with simulated water ingress and copper wire.
9	7	1	Similar to Core 5 with simulated water ingress.
10	8	1	Similar to Core 5 with small quantity of simulated water ingress.
11	9	1	Core 5 with an equal number of fuel and moderator pebbles.
—		*2*	*Reproducibility measurement.*
12	10	1	Similar to Core 9 with simulated water ingress.

Hexagonal Close Packed

Random

Columnar Hexagonal Point-On-Point

Assumptions in Original HTR-PROTEUS Benchmarks

- Limited computing resources to evaluate all uncertainties in detail
- Any uncertainties not unique to a given subset of configurations was not evaluated if the evaluated uncertainty in Cores 1, 1A, 2, and 3 had a 1σ in Δk_{eff} value $\leq$0.00030.
  - The MCNP statistical uncertainty was ~0.00010
  - Dominant uncertainties (i.e. > 100 pcm) were radial reflector graphite density and composition, and ^{235}U enrichment
- Composition and impurity uncertainties were evaluated using min/max of the primary alloy constituent or estimation of an equivalent boron content (EBC)

Revised MCNP Analyses

- MCNP statistical uncertainty 1σ in k_{eff} between 0.00002 and 0.00003
- Contribution of statistical uncertainties towards adjoint calculations <0.00001
- Initial comparison between original MCNP-5.1.60 with ENDF/B-VII.0 direct perturbation and MCNP-6.3.0 with ENDF/B-VII.1 sensitivity calculations
  - See next page for comparison with Core 5
- Waiting for official MCNP ACER release from LANL with ENDF/B-VIII.1 (end of July, 2025)

Comparison of HTR-PROTEUS Core 5 Uncertainty Calculations for Mass, Density, and Composition

Component	Type	1σ in k_{eff} Old	1σ in k_{eff} New
Concrete Shielding	c	NE	0.00002
	ρ	NE	<0.00001
Steel Pedestal Support	c	NE	0.00001
	ρ	NE	<0.00001
Safety Ring	c	NE	0.00004
	ρ	NE	<0.00001
Upper Reflector Support	c	0.00034	0.00022
	ρ	NE	0.00002
Ambient Air	c	NE	0.00006
	ρ	NE	0.00004
Radial Graphite Reflector	c	0.00108	0.00095
	ρ	0.00103	0.00097
Lower Reflector Cylinder	c	NE	0.00012
	ρ	NE	0.00004
Lower Reflector Annulus	c	NE	<0.00001
	ρ	NE	0.00017
Upper Reflector Graphite	c	NE	0.00002
	m	NE	<0.00001
Shutdown Rods Borated Steel	c	NE	<0.00001
	ρ	NE	<0.00001
Shutdown Rods Steel Tube	c	NE	<0.00001
	ρ	NE	<0.00001
Al Shock Dampers	c	NE	<0.00001
	ρ	NE	<0.00001

Component	Type	1σ in k_{eff} Old	1σ in k_{eff} New
TRISO: UO_2 Kernel	c	NE	0.00001
	m	0.00028	0.00029
	ρ	—	0.00067
	^{234}U	NE	0.00018
	^{235}U	0.00233	0.00234
	^{236}U	NE	0.00004
	^{238}U	NE	0.00039
	O:U	NE	<0.00001
TRISO: Buffer Layer	c	NE	<0.00001
	ρ	NE	0.00004
TRISO: IPyC Layer	c	NE	<0.00001
	ρ	NE	0.00003
TRISO: SiC Layer	c	NE	<0.00001
	ρ	NE	0.00001
TRISO: OPyC Layer	c	NE	<0.00001
	ρ	NE	0.00004
Fueled Pebble Matrix	c	0.00014	0.00010
	m	NE	0.00003
	H_2O	NE	0.00013
Unfueled Graphite Layer	c	0.00016	0.00011
	H_2O	NE	0.00006
Moderator Pebble	c	0.00087	0.00050
	m	NE	0.00011
	H_2O	NE	0.00007

Total 1σ uncertainty is still ~300 pcm

Core Center Reaction Rate Ratios for Core 5

Source	k_{eff}	1σ	C8/F5	1σ	F8/F5	1σ	F9/F5	1σ
Benchmark	1.0024	0.0030	--	--	--	--	--	--
Experiment	--	--	3.681E-02	1.0%	3.24E-04	4.5%	2.080	1.2%
ENDF/B-VII.0	1.00724	0.00005	3.65E-02	1.30%	3.95E-04	0.50%	2.02	0.38%
ENDF/B-VII.1	0.99320	0.00005	3.81E-02	1.29%	4.02E-04	0.50%	2.02	0.38%
ENDF/B-VIII.0	1.00205	0.00005	3.68E-02	1.31%	3.93E-04	0.50%	1.92	0.39%
JEFF-3.3	0.99474	0.00005	3.74E-02	1.28%	3.89E-04	0.50%	2.00	0.38%
JENDL-5.0	0.99829	0.00005	3.67E-02	1.34%	3.97E-04	0.50%	1.92	0.38%
TENDL-2021	1.00237	0.00005	3.68E-02	1.32%	3.86E-04	0.50%	1.92	0.38%
Comparison	**Δk_{eff} (pcm)**	**1σ (pcm)**	**C/E**	**1σ**	**C/E**	**1σ**	**C/E**	**1σ**
ENDF/B-VII.0	484	300	0.99	0.02	1.22	0.06	0.97	0.01
ENDF/B-VII.1	-920	300	1.04	0.02	1.24	0.06	0.97	0.01
ENDF/B-VIII.0	-35	300	1.00	0.02	1.21	0.05	0.92	0.01
JEFF-3.3	-766	300	1.02	0.02	1.20	0.05	0.96	0.01
JENDL-5.0	-411	300	1.00	0.02	1.23	0.06	0.92	0.01
TENDL-2021	-3	300	1.00	0.02	1.19	0.05	0.92	0.01

30% porosity →

20% porosity → ENDF/B-VIII.1 $k_{eff} = 1.00147 \pm 0.00003$

$\Delta k_{eff} = -93 \pm 300$ pcm

HTR-PROTEUS ~22-25 % POROSITY

Subcritical Measurement Data

- Subcritical measurements were performed on Cores 1, 5, and 7
- Evaluation of these data would enhance validation for subcritical storage/transport of TRISO-laden fuel pebbles
  - Cores 1 and 5 represent different PFs
  - Cores 5 and 7 compare water ingress effects
- The challenge is to determine whether sufficient information is available regarding the detector systems, and their placement, to provide quality benchmark evaluation data

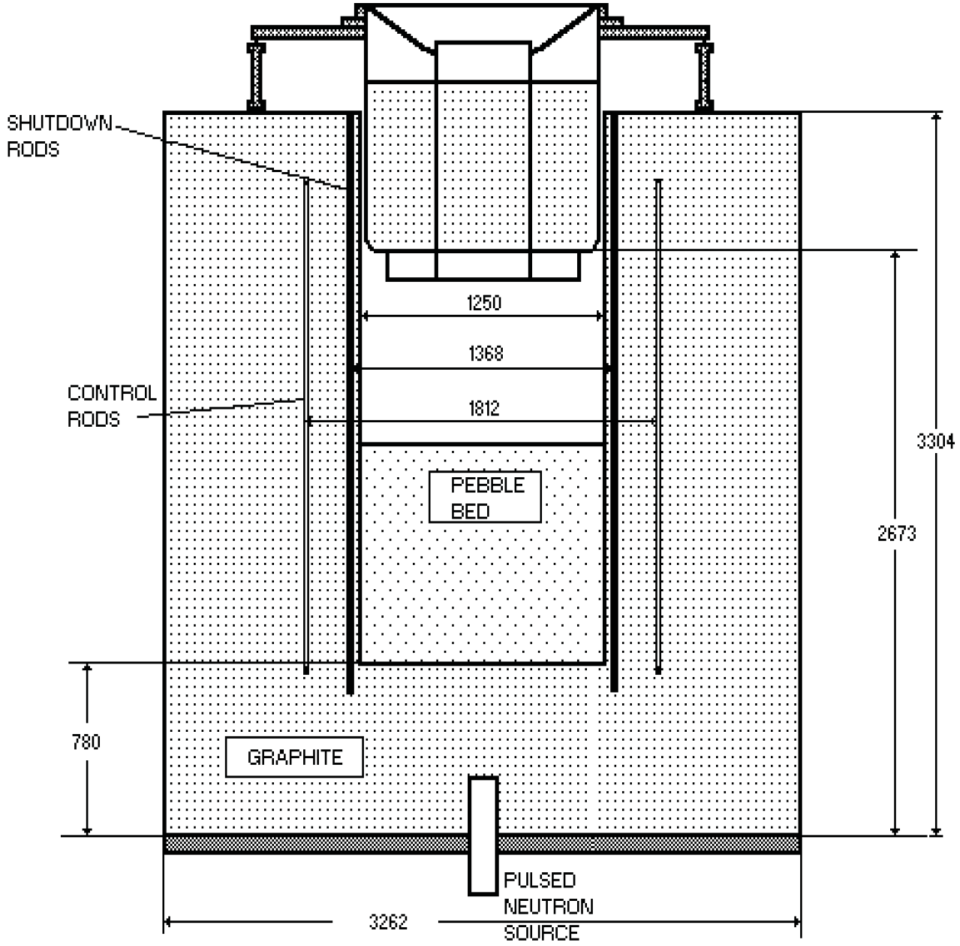
Remaining Data for Benchmark Evaluation

	CRITICAL LOADING	Σ_a	SUBCRIT CORE	SHUTDOWN RODS		CONTROL RODS		UPPER REFL.	β/Λ	MEAS. RODS	CENT. CONT. ROD	TEMP. COEFF	COM-PONENT WORTHS	MISC.	REACTION RATE DISTRIBUTIONS					REACTION RATE RATIOS		
															IN CORE			IN PEBBLE		AT CORE CENTRE		
METHOD / CORE	PEBBLE COUNT	PNS	PNS	PNS	IK	SP	PNS	PNS (SP)	PNS	PNS	PNS	COMP	COMP	-	FOILS	FISSION CHAMBER.	γ SCAN	FOILS	PARTICLE FOILS	FOILS	PARTICLE FOILS	WHOLE PEBBLE
G1		✓													F: 5 C: 8	F: 5, 8, 7, 9, 2, 1						
1	✓		✓	✓	✓	✓	✓		✓	✓			✓		F: 5, 8 C: 8	F: 5, 8, 7						
1A	✓				✓	✓										F: 5, 8, 7						
2	✓			✓	✓	✓	✓	✓	✓						F: 5, 8 C: 8	F: 5, 8, 7						
G2		✓														F: 5, 8						
3	✓		✓	✓	✓	✓	✓		✓													
1A	✓			✓		✓																
4(1)	✓					✓																
4(2)	✓			✓	✓	✓																
4(3)	✓			✓		✓																
5	✓			✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	water/ CH_2 CH_2 in lower axial reflector	F:5,8 C8	F:5,8,7	C8, Ftot	F:5,8,9 C8	Ftot C8	F:5,8,9 C8	C8/Ftot	C8/Ftot
6	✓					✓																
7	✓			✓	✓	✓	✓	✓	✓	✓	✓	✓		water/ CH_2 CH_2 in lower axial reflector	F:5,8 C8	F:5,8,7	C8, Ftot	F:5,8,9 C8	Ftot C8	F:5,8,9 C8	C8/Ftot	C8/Ftot
8	✓						✓															
9	✓				✓	✓	✓	✓	✓	✓					F:5	F:5,8,7,9	C8, Ftot	F:5,8,9 C:8				
10	✓		✓		✓	✓	✓	✓	✓	✓				subcriticality with CH_2 removed	F:5	F:5,8,7,9	C8, Ftot	F:5,8,9 C:8				

✓ F: 5 = PLANNED AND EXECUTED

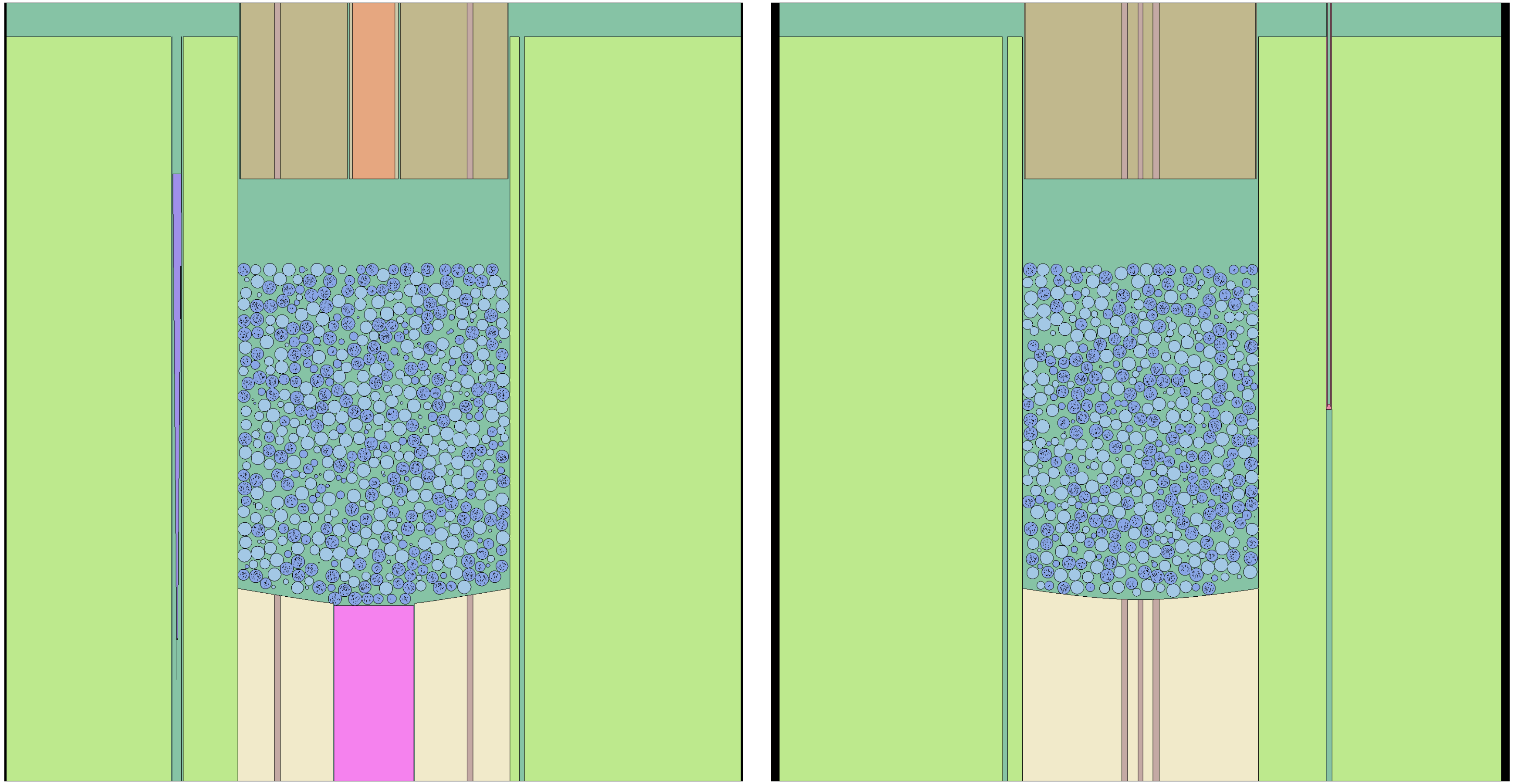
F=fission, C=capture, 5=U-235, 8=U-238, 9=Pu-239, 7=Np-237, 2=Pu-242, G1,2=graphite (no fuel in core), COMP. = compensation with calibrated control rods

CORE 4



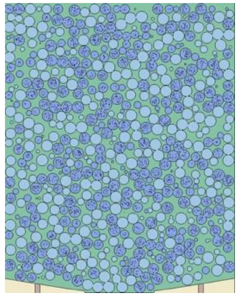
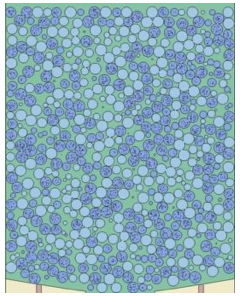
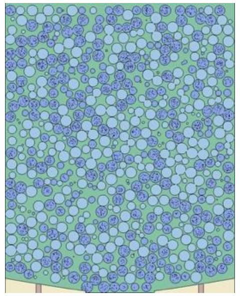
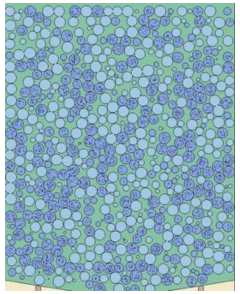
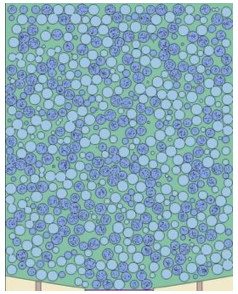
- Random packing
- Safety/Shutdown rods all out
- Withdrawable control rods and auto-rod in use
- 1:1 fuel-to-moderator pebble ratio
- 3 different randomly loaded cores

Core 4: Serpent Model



Random Packing Distributions

- OpenMC and Project Chrono were used to generate random pebble positions
- 50 OpenMC purely random positions for Core 4.2 (and 4.3)
- 60 Project Chrono DEM random pebble positions for Core 4.2 (and 4.3)
- Core 4.2
  - Core height 152cm
  - 4940 moderator
  - 4940 fuel
  - Total of 9880

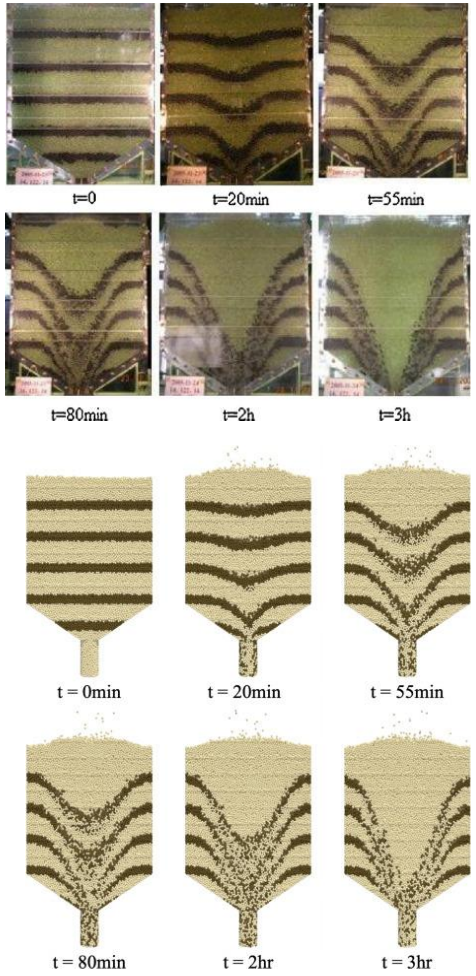






+105

Project Chrono

- DEM uses Newton's laws of motion to determine the linear and rotational movement of particles
- GPU-based (high performance compared to CPU equivalent)
- A major assumption in DEM is that particles are permitted to have small amounts of intersection at points of contact (u_n)
- This intersection is then used to compute the normal and tangential (friction) forces between particles using a spring-dashpot mechanism
- Another assumption is that all pebbles have the same density which is an average between fuel and moderator pebbles
- To accelerate the simulation, pebbles are dropped as "sheets" into the vessel, with positions within the sheet randomly assigned.

Parameter	Value
Sphere Density	1.736 g/cc
Elastic Modulus	8 GPa
Poisson's Ratio	0.12
Sliding Friction Coefficient	0.3
Rolling Friction Coefficient	0.01

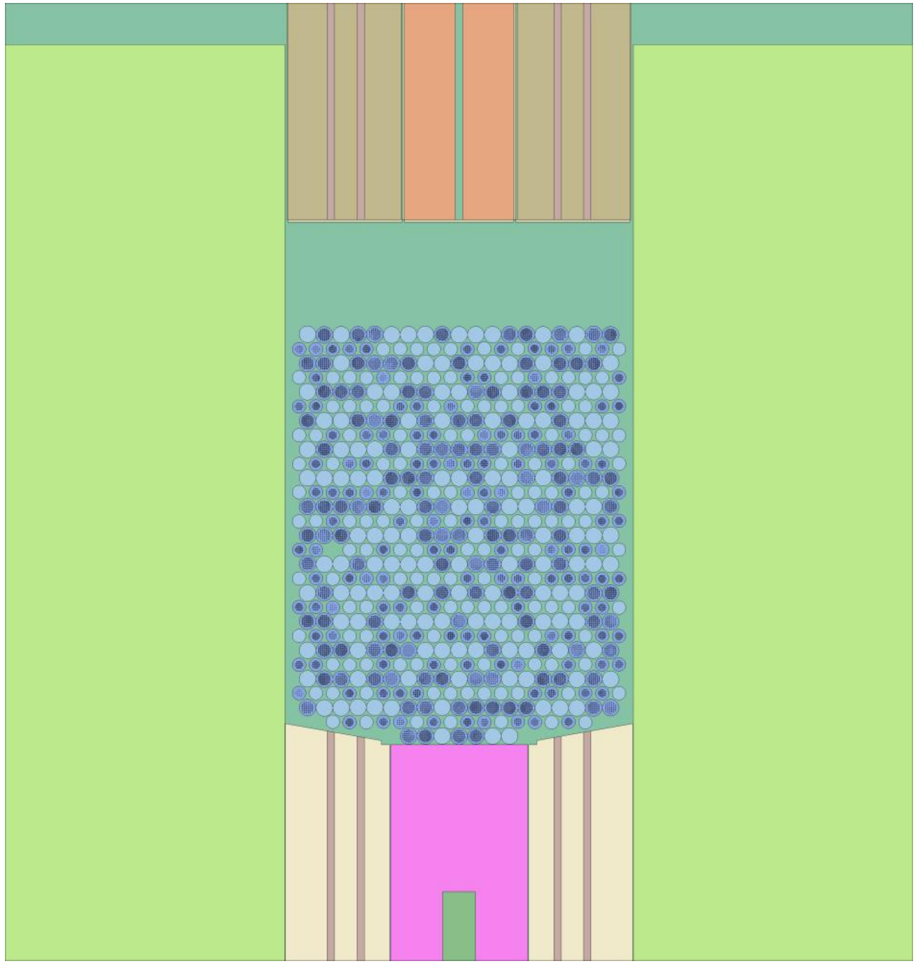


David Reger, et al.,"Discrete element simulation of Pebble Bed Reactors on graphics processing units," Ann. Nuc. Ene.,Vol. 190, 2023.

Verification of the Serpent model

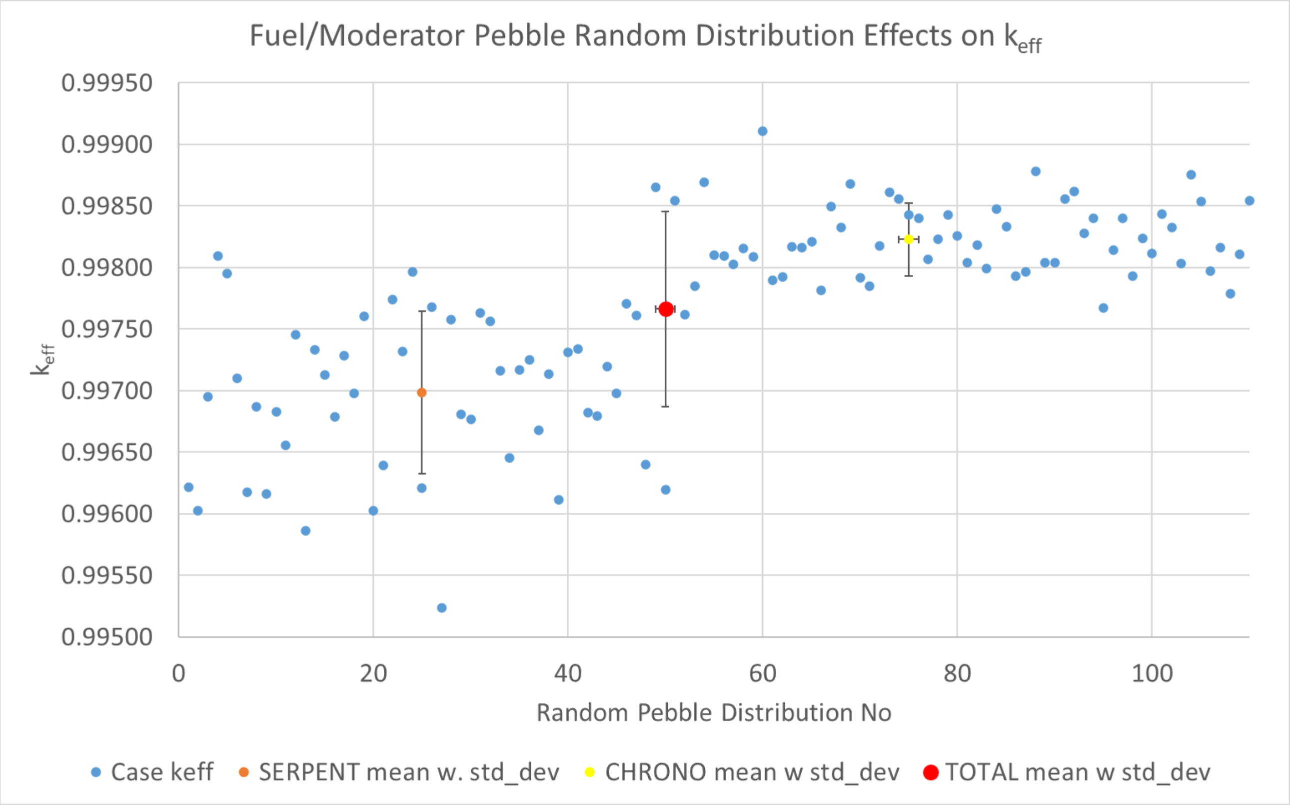
- IRPhEP Core 4 model were modeled with Serpent and compared to the published MCNP model result.
- MCNP 6.1
- ENDF/B VII.1 library

	keff	std. dev.
MCNP 6.1	1.00266	0.00007
Serpent	1.00276	0.00004
Difference (pcm)	10	



Serpent k-eff Analysis for Core 4.2

- Version 2.1.32
- ENDF/B VII.1 XS Library
- Run params:
  - 500,000 n/cycle
  - 300 skipped cycles
  - 1000 active cycles



Distribution	MEAN	VARIANCE	Standard Deviation
OPENMC (50)	0.996985	4.37576E-07	0.00066
Project CHRONO (60)	0.998228	8.81398E-08	0.00030
TOTAL	0.997663	6.30038E-07	0.00079

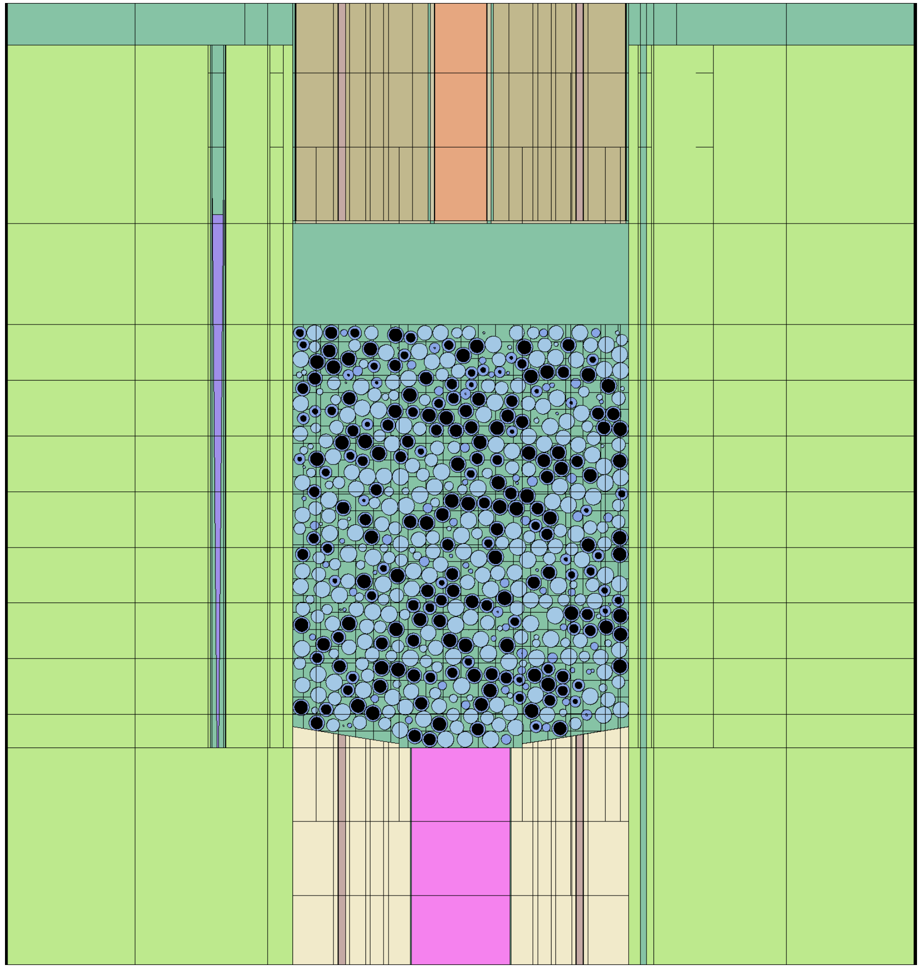
Preliminary Rod Worth Analysis with Serpent

	Experiment		Serpent w. OpenMC Dist.			Serpent w. Chrono Dist.		
ROD No	Worth($)	Worth(pcm)	Worth($)	WORTH(pcm)	Diff(PCM)	Worth($)	WORTH(pcm)	Diff(PCM)
1	0.407	294	0.360	250	-44	0.382	265	-29
2	0.345	249	0.370	257	8	0.354	246	-3
3	0.330	239	0.369	256	18	0.369	256	18
4	0.383	277	0.370	257	-20	0.359	249	-28
Total	1.465	1059	1.469	1021	-39	1.463	1017	-42

- Preliminary: Rod worth is calculated from the k-eff when the rod of interest is in and out while all the other rods are at their original positions.
- Worth statistical uncertainty = 0.004$

XS Generation for Deterministic Calculations

41					112				
					58	68	80	90	102
42		43			58	69	80	91	102
44	45	46	47	48	58	70	80	92	102
49					59	71	81	93	103
1	9	17	25	33	60	72	82	94	104
2	10	18	26	34	61	73	83	95	105
3	11	19	27	35	62	74	84	96	106
4	12	20	28	36	63	75	85	97	107
5	13	21	29	37	64	76	86	98	108
6	14	22	30	38	65	77	87	99	109
7	15	23	31	39	66	78	88	100	110
8	16	24	32	40	67	79	89	101	111
50	51	52	53	54					
55		56							
57					113				



- Full core Serpent model
- 113 homogenized regions to cover the entire core
- 4G/8G/14G cross-sections

Preliminary Analysis with Griffin and AGREE

- Griffin 2D (R-Z) and 3D core
  - Diffusion
  - Transport (SN)
- AGREE 2D (R-Z) core
  - Diffusion
- Lieberoth steaming correction in the core
- No upper cavity special treatment (air) for diffusion

	k-eff	DIFF (pcm)
SERPENT	1.00173	
AGREE-2D-4G	1.00924	751
AGREE-2D-8G	1.00551	378
AGREE-2D-14G	1.00500	327
GRIFFIN-3D-4G-DIFFUSION	1.00890	717
GRIFFIN-3D-8G-DIFFUSION	1.00458	285
GRIFFIN-3D-14G-DIFFUSION	1.00402	229
GRIFFIN-3D-4G-TRANSPORT	1.01155	982
GRIFFIN-3D-8G-TRANSPORT	1.00149	-24
GRIFFIN-3D-14G-TRANSPORT	1.00006	-167

* Griffin 2D results compare closely to 3D

Conclusion

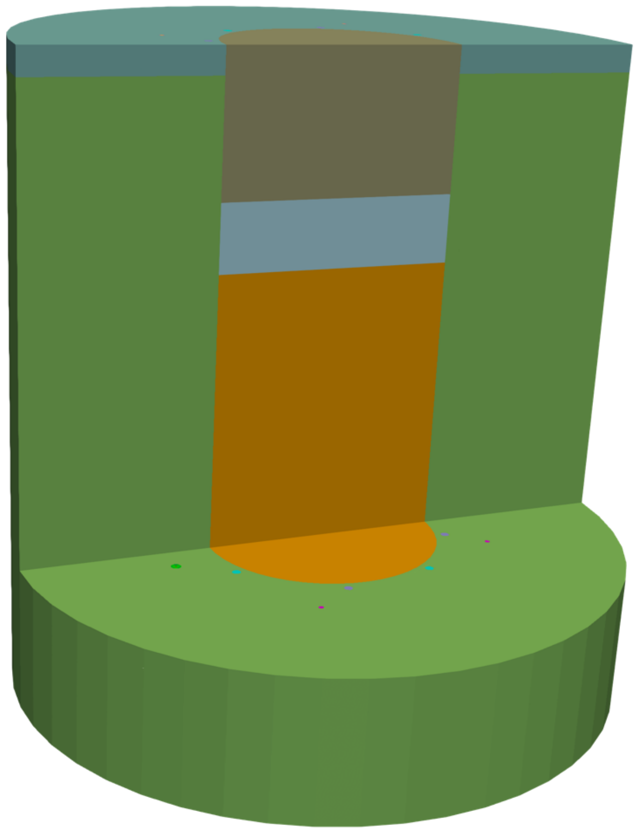
- Started integration of the ICSBEP report IEU-COMP-THERM-TBD
- Initial results show that MCNP and Serpent agree within 10 pcm for current IRPhEP Core 4 model
- Pebble packing with Project Chrono provides a lower uncertainty in k_{eff} & improved C/E
- Minor updates to sensitivity analysis
- Further investigate the effect from
  - top aluminum safety ring
  - newer nuclear data libraries (TSLs & SANS data)
- Perform additional sensitivity analysis
- Identify, and if possible, evaluate, subcritical measurement data

Acknowledgements

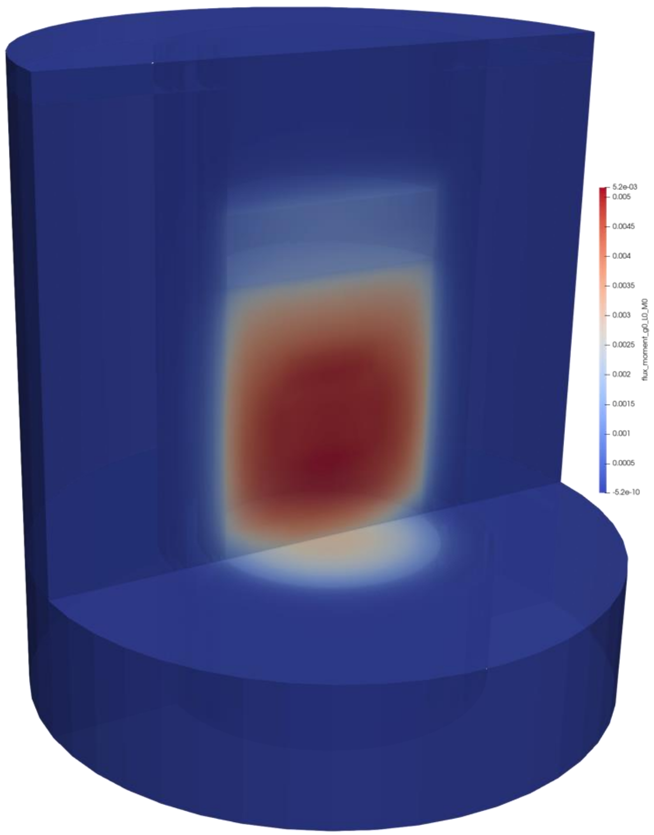
- We would like to thank the following for their support
  - Zachary Bevans (INL intern)
  - Spencer Ercanbrack (INL intern)

ADDITIONAL SLIDES

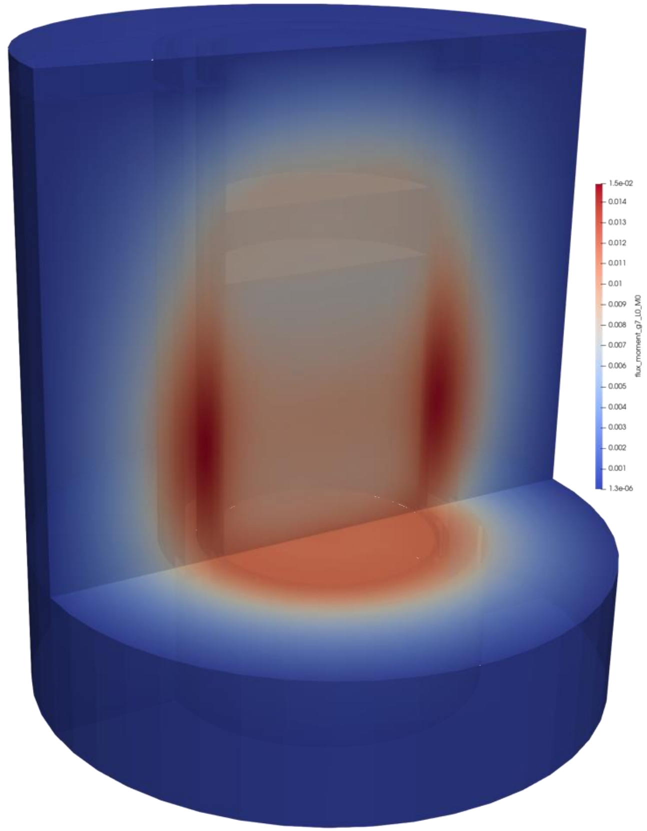
Griffin 3D Core Model



Material mesh

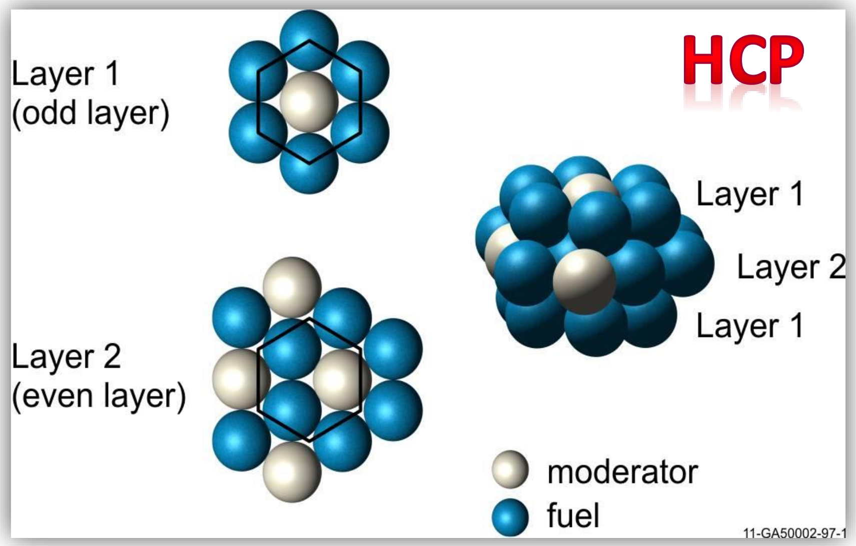


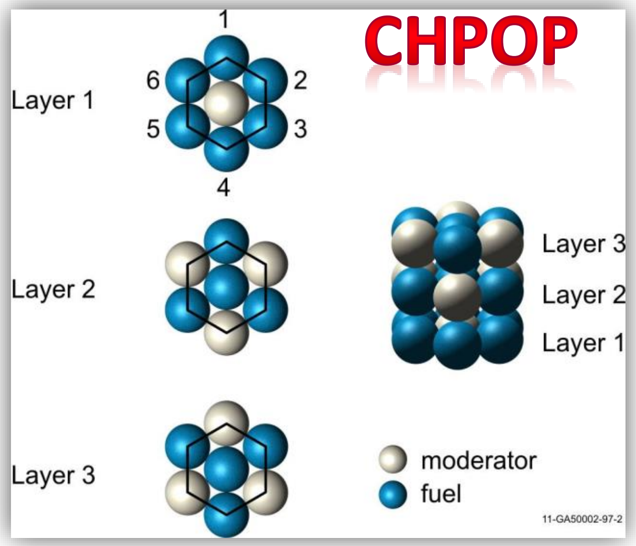
Fast scalar flux (G=1)



Thermal scalar flux (G=8)

Packing Fractions (PFs)





- Hexagonal Close Packed (HCP)
  - 0.7405 theoretical PF (away from edges)
  - ~0.692 core-averaged PF
  - Worst case for shipping/storage accidents
- Random Packing
  - ~0.61 PF
  - Real world is between 0.60 and 0.64
- Columnar Hexagonal Point-On-Point (CHPOP)
  - 0.6046 theoretical PF (away from edges)
  - 0.5835 core-averaged PF
  - Best representation of real world using known pebble locations