Department of NUCLEAR ENGINEERING

2018 SCALE Users' Group Workshop

NCSU activities on High Temperature Reactor Design using SCALE

Oak Ridge National Laboratory

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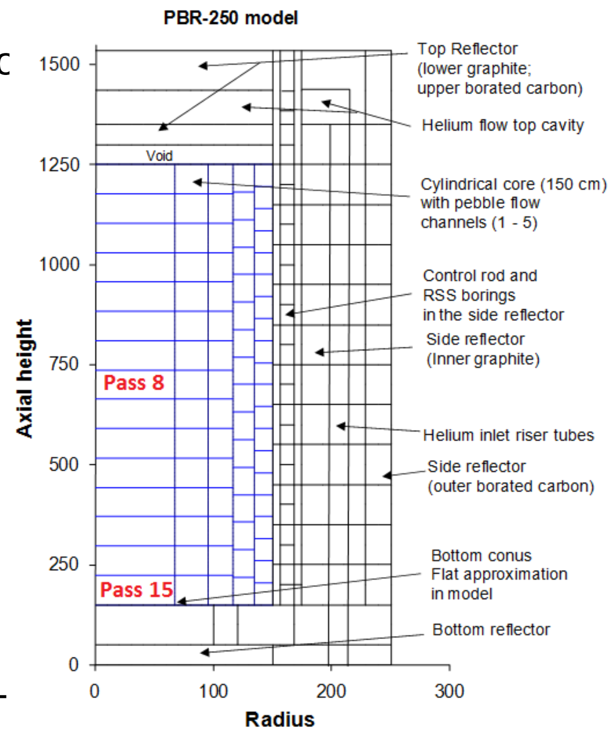
Overview of the ongoing activities

- PBR-250
  - IAEA Coordinated Research Program (CRP) on the HTGR Uncertainty Analysis in Modeling (UAM) - Benchmark Phase I Results (PBR-250),
- MTGR-350:
  - Comparison of the multiplication factor with KENO/SERPENT in single block, super cell and core models,
  - Super cell model spectrum comparison for cross section generation,
  - Space time convergences of the models – NEWT vs KENO/SERPENT

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

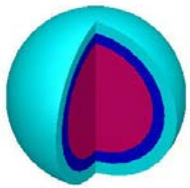
- **Core configurations**
  - Prismatic
  - Pebble bed: representative 250 MWth Pebble Bed Reactor design (PBR-250)
- **Objectives (following ideas of NEA/OECD UAM on LWRs)**
  - To subdivide system into steps
  - To identify inputs, outputs and propagated uncertainties fc each step
  - To calculate resulting uncertainty in each step
  - To propagate the results in integral system
- **In the current study, focuses have been placed on**
  - Exercise I-1 and I-2
  - HTGR modeling options
  - Nuclear data uncertainty
- **Scale version data and modules:**
  - SCALE 6.1, 6.2, 6.2.2,
  - KENO-VI, TSUNAMI-3D
  - ENDF/B VII.0, ENDF/B VII.1, 44groupcov, 56groupcov7.1

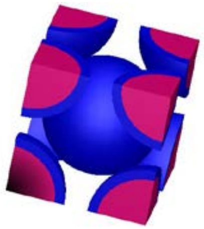


Benchmark Phase I: local standalone neutronics simulation

- 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	

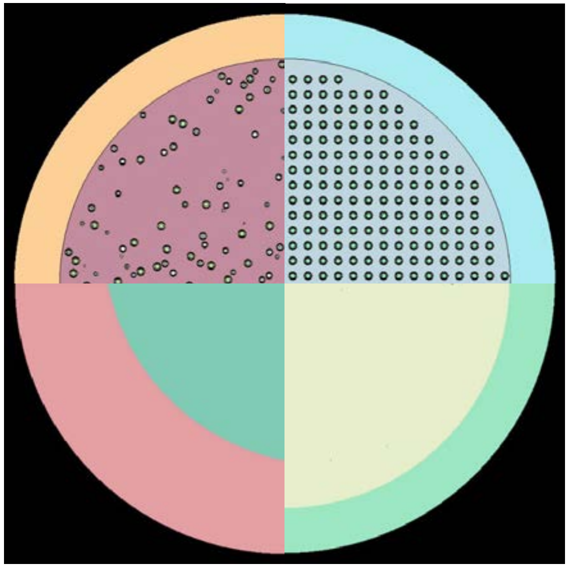
* 4.2% is the fuel enrichment usually used in HTGR criticality in fresh core

† Burn-up of this representative fuel sphere is ~63,000 MWd/T

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]
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
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: Δk < 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):

- Relatively large difference between ENDF/B-VII.0 and -VII.1
- Effect on criticality calculation ~200 pcm for a coated particle ~1100 pcm for a core unit.

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

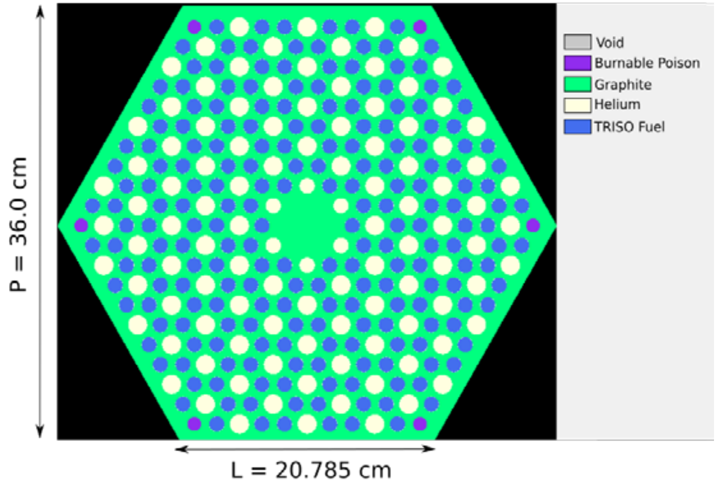
No.	8.9%wt		4.2%wt	
	Matrix	Contribution	Matrix	Contribution
1	U-235 $\bar{\nu}$	3.7866E-01	U-235 $\bar{\nu}$	3.8136E-01
2	U-235 (n,γ)	2.0919E-01	U-238 (n,γ)	2.2987E-01
3	U-238 (n,γ)	1.6196E-01	U-235 (n,γ)	1.9664E-01
4	U-235 $(n,f)(n,\gamma)$	1.0949E-01	Graphite (n,γ)	1.7274E-01
5	Graphite (n,γ)	9.0193E-02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

Comparison of the multiplication factor with KENO/SERPENT in single block, super cell and core models

Objectives:

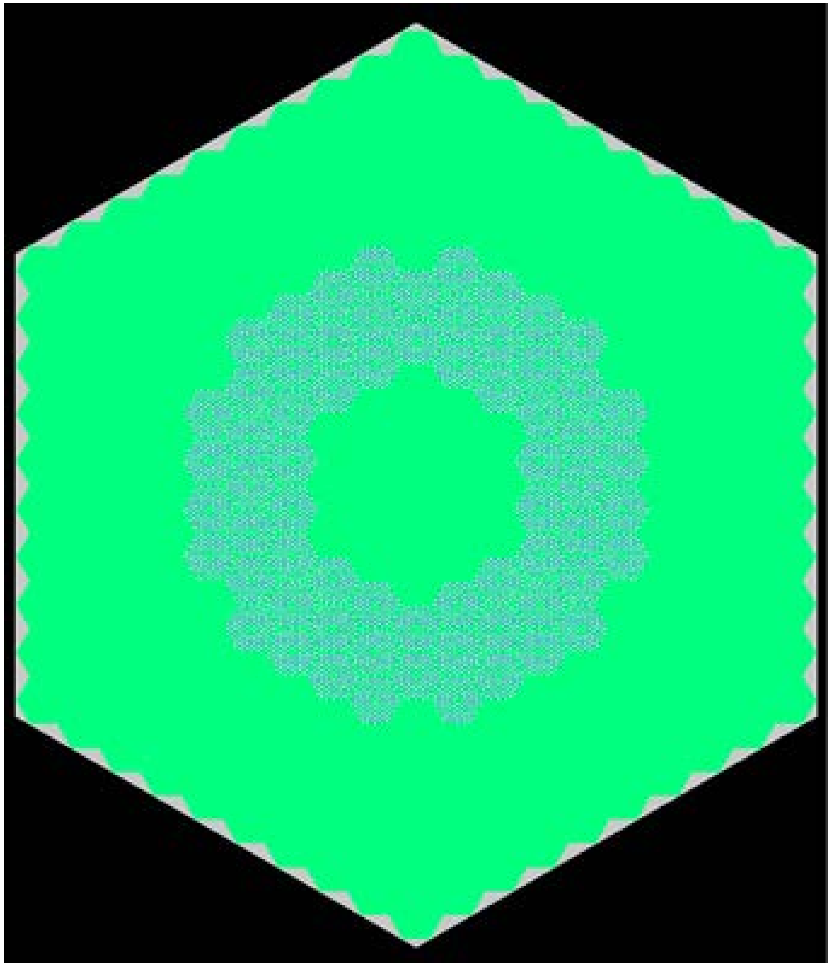
- Comparing criticality calculation between SERPENT2 and SCALE-6.2.0/KENO-VI
- Evaluating the effect of CE vs MG structure

Models Description

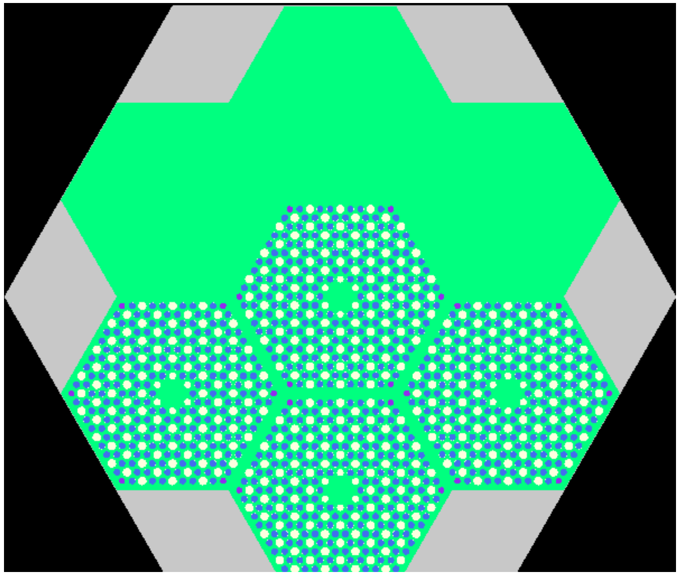


Single block

Core



Super cell



Criticality calculations

Compact cell

Model	k-infinity	Std Deviation (pcm)	Abs difference (pcm)
SERPENT-CE	1.25772	22	Reference
KENO-CE	1.25829	64	57
KENO-252MG	1.24567	61	1262
NEWT-252MG	1.24134	-	1638

Fuel block

Model	k-infinity	Std deviation (pcm)	Abs ifference (pcm)
SERPENT-CE	1.06605	7	Reference
KENO-CE	1.06632	73	27
KENO-252MG	1.06213	62	-392

Super cell

Model	k-infinity	Std deviation (pcm)	Abs difference (pcm)
SERPENT-CE	1.08670	7	Reference
KENO-CE	1.08813	70	143
KENO-252MG	1.08362	58	-308

Full core

Model	k-infinity	Std deviation (pcm)	Abs difference (pcm)
Serpent-CE	1.06641	22	Reference
KENO-CE	1.06732	70	91
KENO-252MG	1.06237	67	404

Conclusions

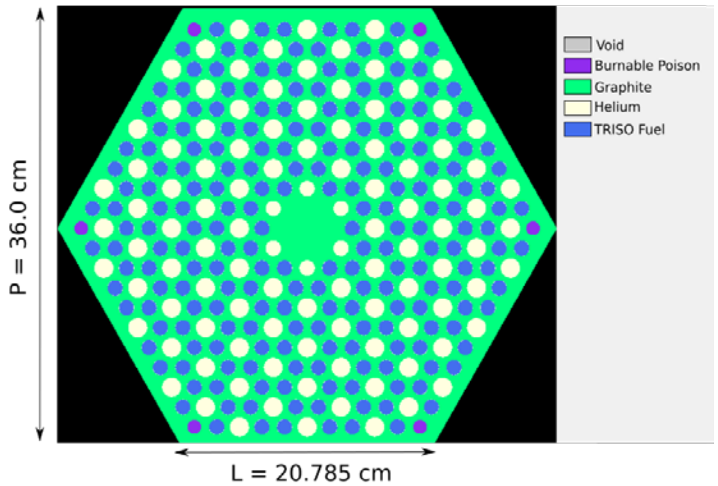
- As expected the continuous energy mode is in better agreement than the multi-group mode results for all of the models.
- The multi-group calculations underestimate the multiplication factor by ~400 pcm. The Serpent and KENO-CE simulations agree within 2 standard deviations.

Super cell model spectrum comparison for cross section generation

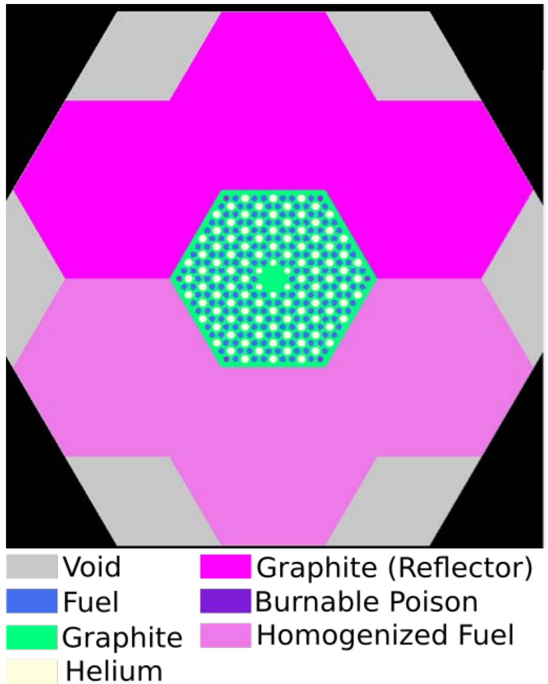
Objectives:

- Providing a reference spectrum from serpent and comparing it with NEWT.
- Comparing the core flux spectrum to different super cells to get the configuration that reproduce the core wide spectrum better to generate 26-group libraries for the PHISICS/RELAP5-3D model using NEWT.

Presentation of the models

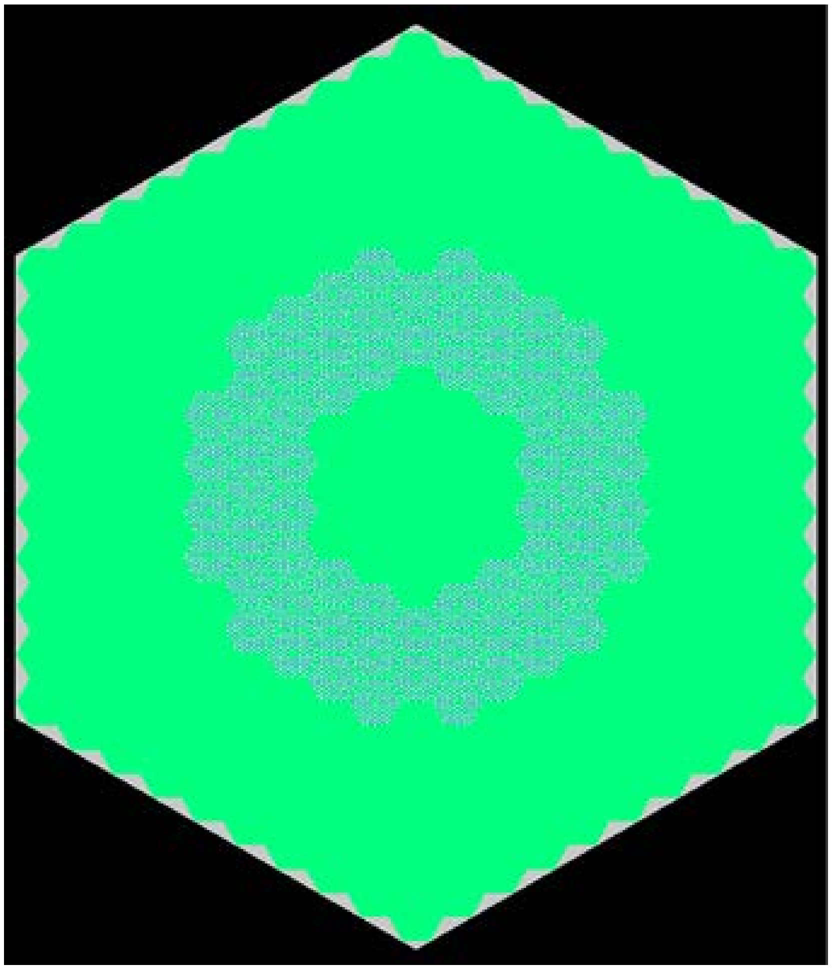


Single block

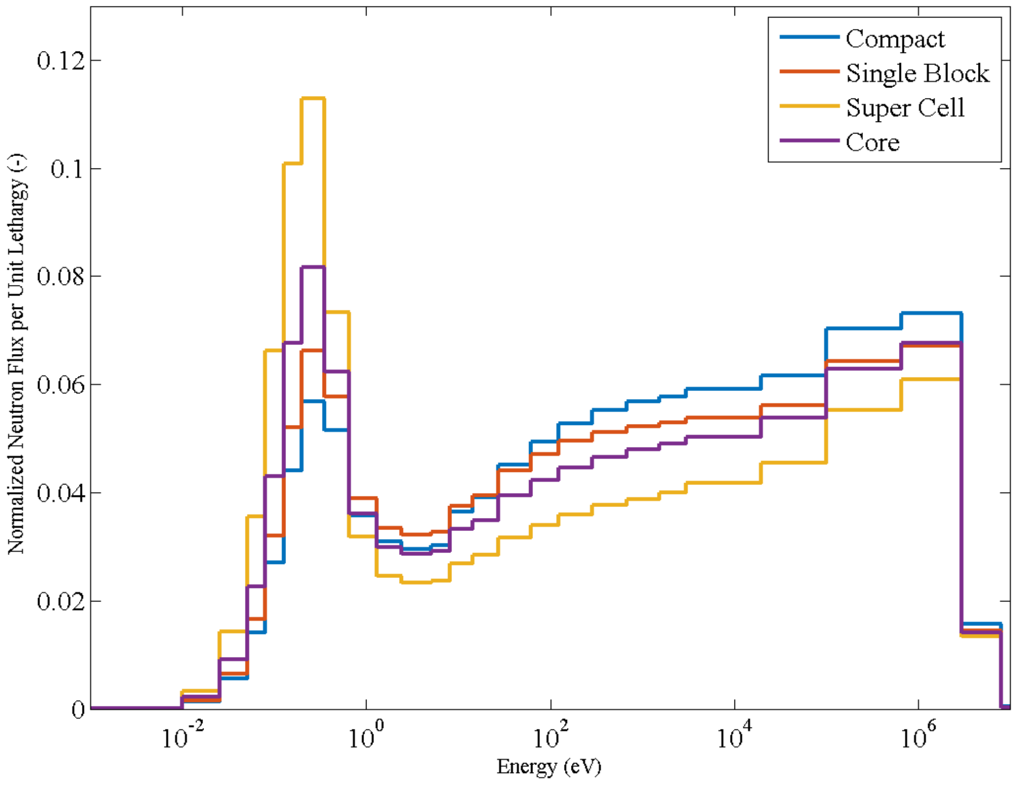


Super cell

Core



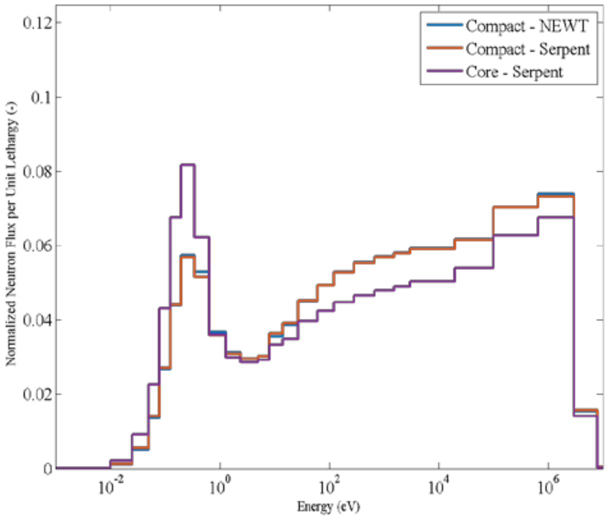
Variation of neutron flux spectrum in various sub-models



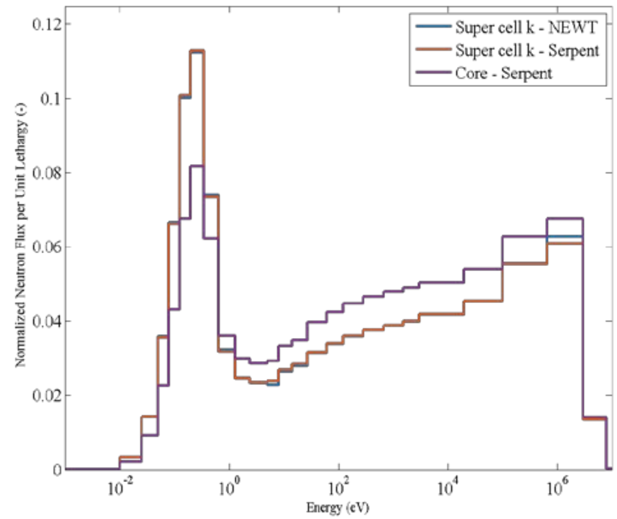
Overview of the SERPENT neutron flux spectra in the various sub-models representative of MHTGR analysis

Comparison of the neutron flux spectra between Serpent and NEWT

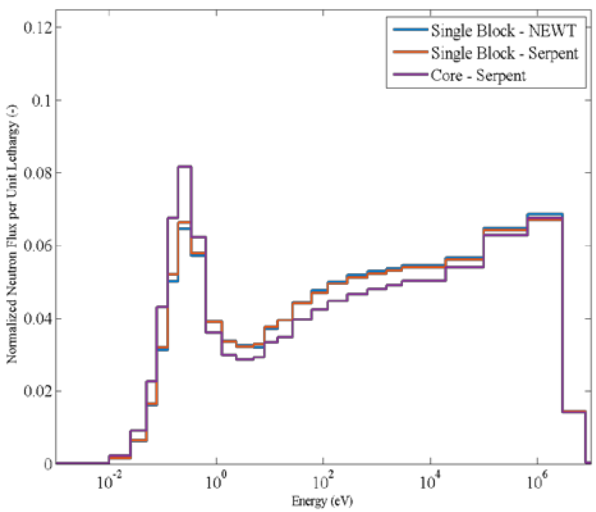
Compact



Super cell

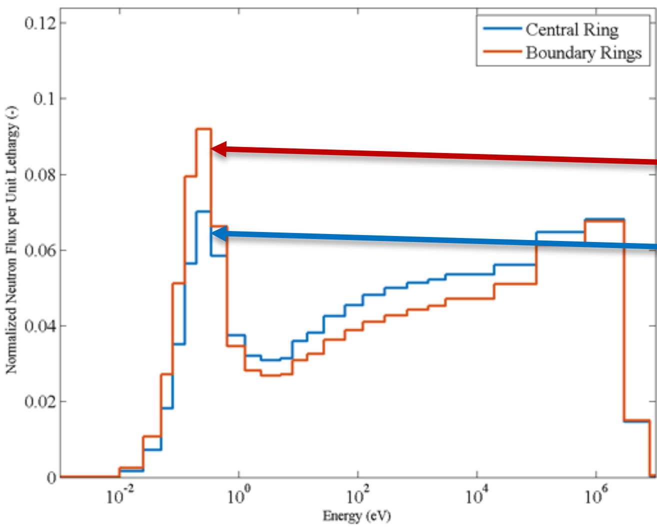


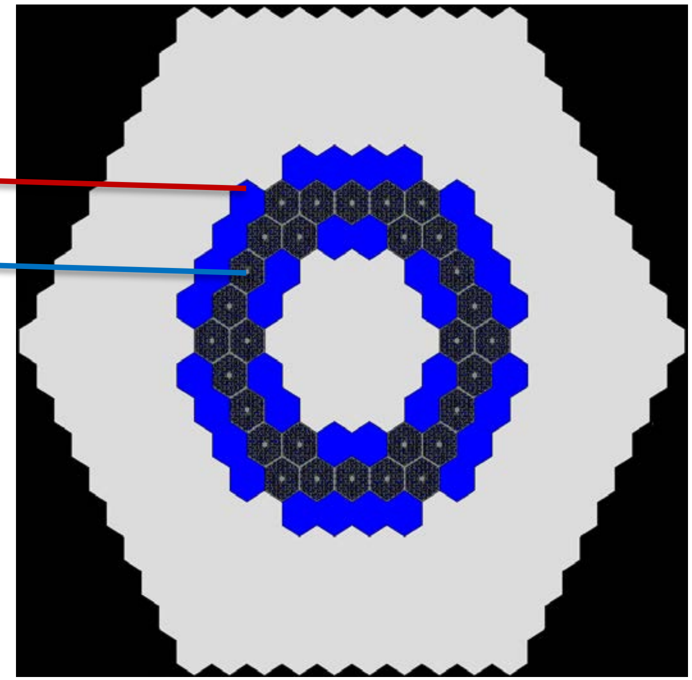
Single block



- Good agreement between NEWT and Serpent in any models
- Super cell with 3 graphite blocks too soft, single block too hard

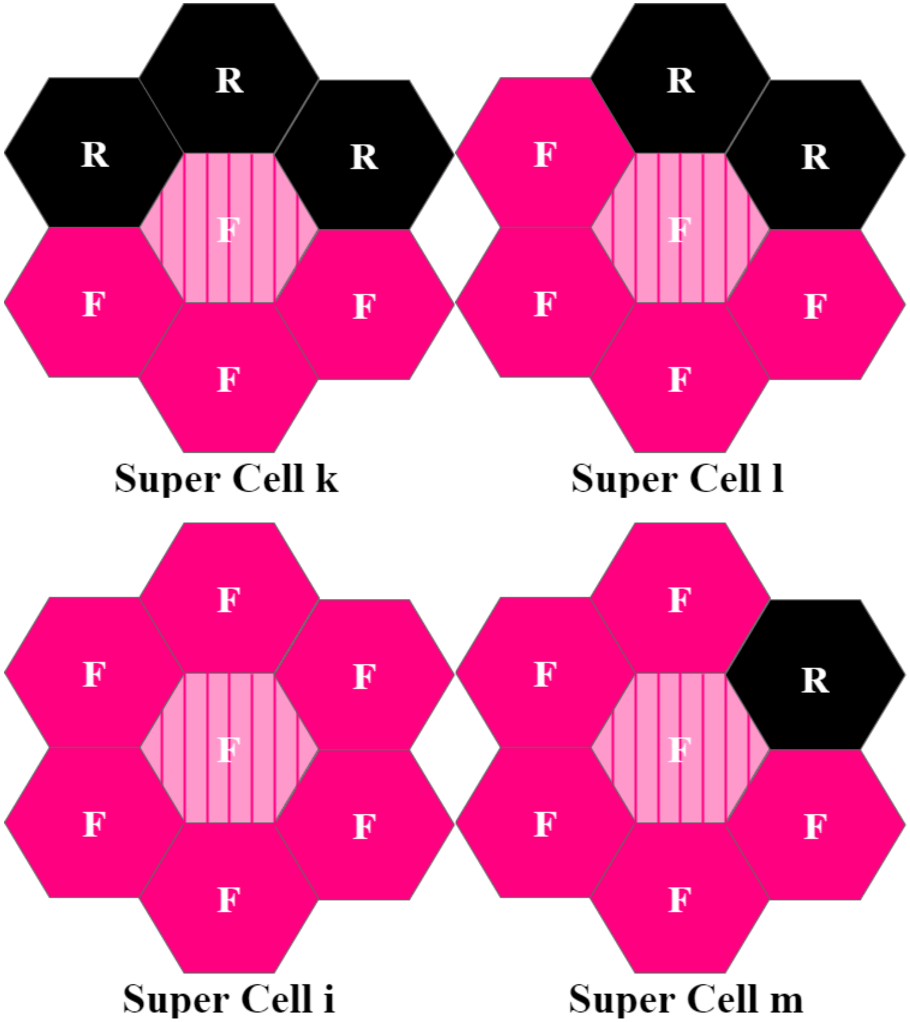
Neutron flux spectrum across the core





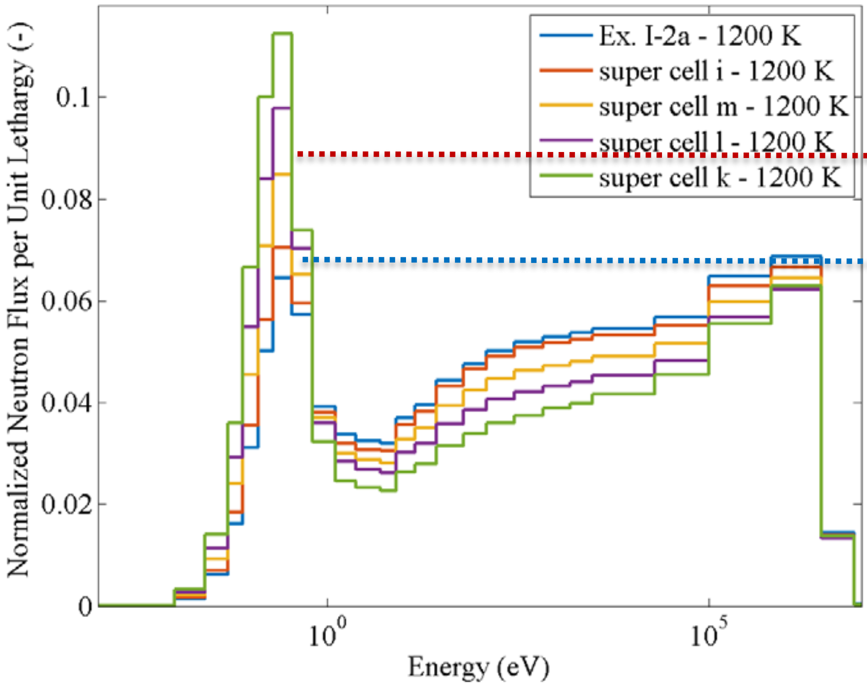
- In the core outer and inner rings: soft spectrum
- In the core central region: harder spectrum comparable to single block

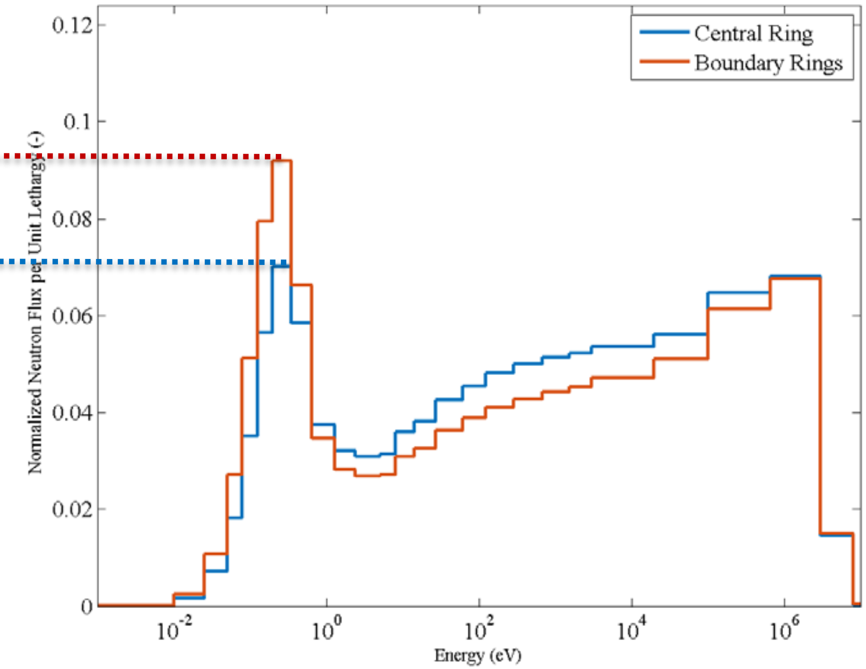
Reminder on the super cell designs



- Pink Striped = heterogeneous block (fresh fuel)
- Plain pink = homogenized fresh fuel
- Plain black = homogeneous graphite (moderator)
- **Flux is only evaluated in the heterogeneous region (center)**

Comparison of the super cell spectra and core local spectra





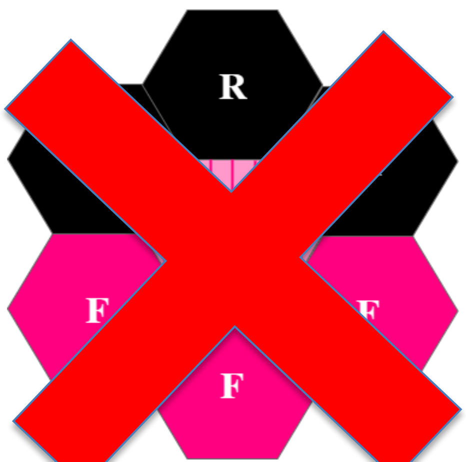
The super cell m has an equivalent spectrum to the global core spectrum

The super cell l (or m) has an equivalent spectrum to the spectrum on the inner and outer ring of the core

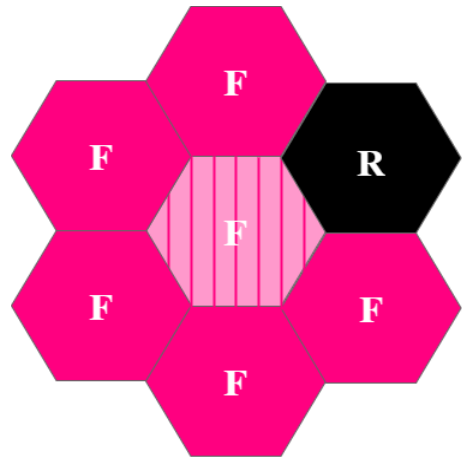
The single block has an equivalent spectrum to the central ring of the core

Conclusions

The best supercells to be used in the benchmark are:

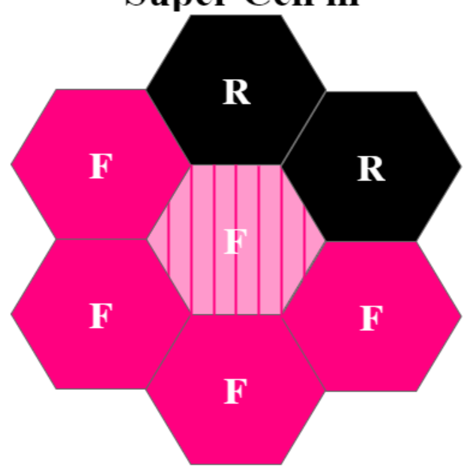


Super Cell k



Super Cell m

or



Super Cell l

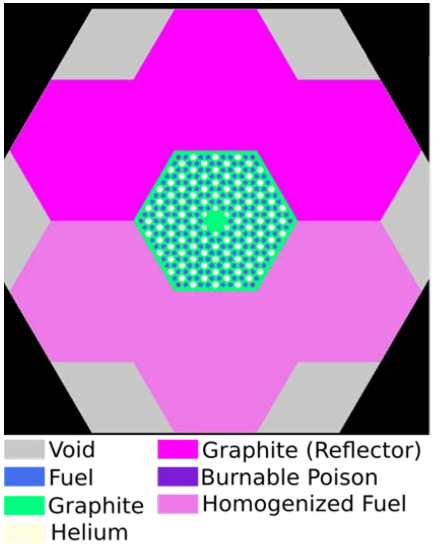
Space time convergences of the models – NEWT vs KENO/SERPENT

Objectives:

- Giving an overview of running time and general convergence of the various models,
- Show that the NEWT models converge to KENO or Serpent results as the parameters are refined,
- Give an order of magnitude of sensitivity of the refined parameter,
- Recommend specifications for the depletion exercises

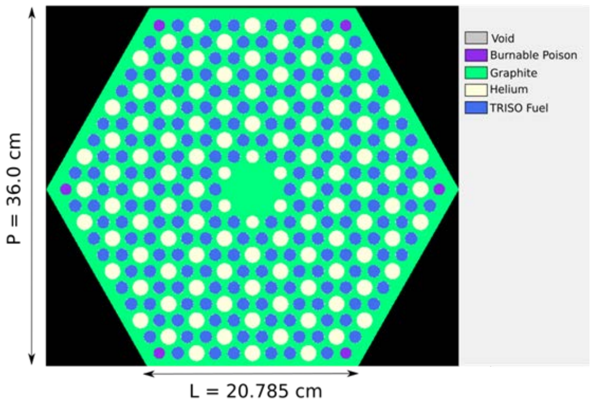
NEWT convergence parameters

- Define default values and refine systematically one parameter:
  - Number of polar angles (**default: 3**) and azimuthal angles (default: **3**)
  - Pn Scattering order: **1**
  - Spatial grid: **24x24** for a given block



- One super cell with graphite (labelled "k")
- One super cell with fuel only (labelled "i")
- Super cell with one homogenized region

Single block



Results on multiplication factor

Discretization	Ex. I-2a	Super cell i	Super cell k
12x12	-	1.18549	
24 x 24	*1.02011*	*1.18576*	*1.25946*
48 x 48	1.02013	1.18590	1.25703
96 x 96	1.02001	1.18595	1.25606
192 x 192	1.02000	-	-
$P_N = 1$	1.02011	1.18576	1.25946
$P_N = 3$	1.02014	1.18577	1.25945
$P_N = 5$	1.02014	1.18577	1.25945
$N_{AZ} = 3$	1.02011	1.18576	1.25946
$N_{AZ} = 6$	1.02054	1.18568	1.25949
$N_{AZ} = 9$	1.02107	1.18572	-
KENO ref	1.02242	1.18677	1.25523

Grey: less than 10 pcm difference to the reference
Purple: Default model results
Red: more than 200 pcm difference

Results on neutron flux spectra

The difference in the neutron flux spectra in the 26 energy groups are evaluated as the parameters are refined

- **P_N**

Average difference: < 0.01 %

Maximum difference: 0.01 %

- **Grid**

Average difference: 0.09 %

Maximum difference: 0.28 % (group 26)

- **N_{AZ}**

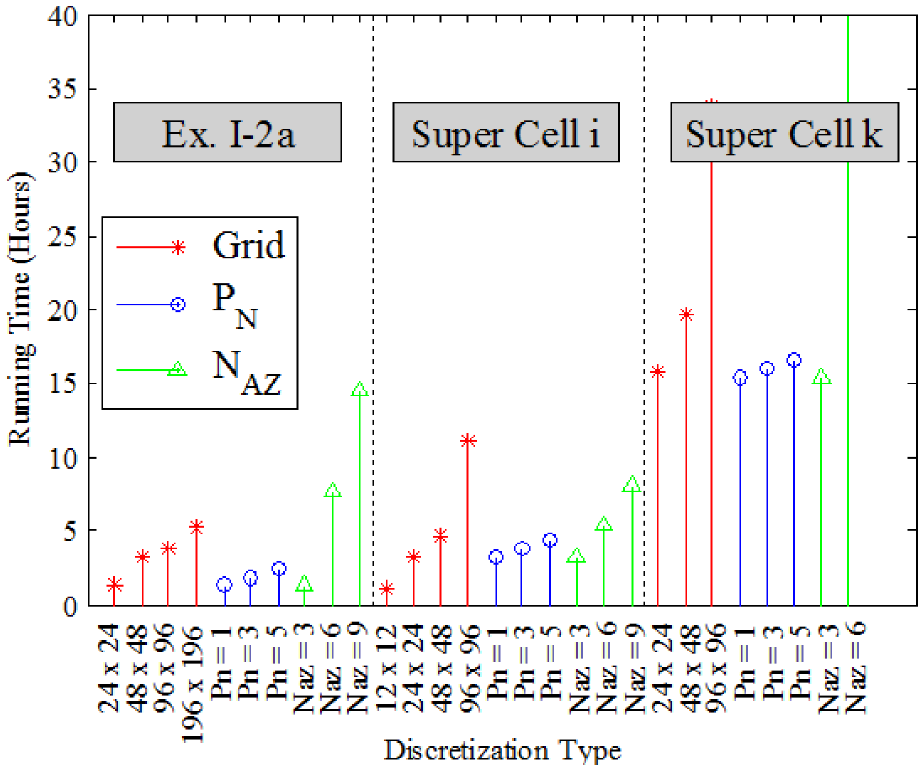
Average difference: -0.03 %

Maximum difference: 0.09 % (group 26)

Comments on the results

- The P_N order has no influence on the multiplication factor. Does not change the flux
- The grid
  - negligible changes in heterogeneous region (< 10 pcm)
  - Large changes as the graphite is refined (~200 pcm)
  - Minor changes in heterogeneous fuel (~30 pcm)
  - Minor changes in the flux
- Number of azimuthal angles
  - Negligible effect in homogeneous regions
  - Medium effect in heterogeneous regions
  - No effects on the flux

Running time



P_N: inexpensive, but no influence
N_{az}: expensive, medium influence
Grid: expensive and influent

More influence of the grid in non-multiplying media regions, in terms of output and running time

Configuration chosen for criticality calculations

Region	Discretization
Heterogeneous block	24 x 24 grid
Homogenized fuel	24 x 24 grid
Graphite	48 x 48 grid
P_N order	1
N_{AZ}	3

Model	k_{inf} NEWT	k_{inf} KENO-VI [std dev in pcm]	Absolute diff. (pcm)
Ex. I-2a	1.02011	1.02242 [15]	-231
Super cell i	1.18576	1.18677 [13]	-101
Super cell m	1.2571	1.25730 [16]	-20
Super cell l	1.33136	1.33063 [14]	73
Super cell k	1.25703	1.25523 [14]	180

Thanks for your Attention!