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Serpent User Group Meeting October 27-30, 2020

Serpent2/POLCA8 3D Single-Channel Benchmark

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Presentation Layout

- Background
- Benchmark Configuration
- 2D Lattice Physics Calculations and XS Generation
- Serpent2 3D Reference Calculations
- POLCA8 Calculations
- 2D Lattice Physics Results
- 3D Simulation Results
- Summary of Main Observations
- Conclusions and Future Work

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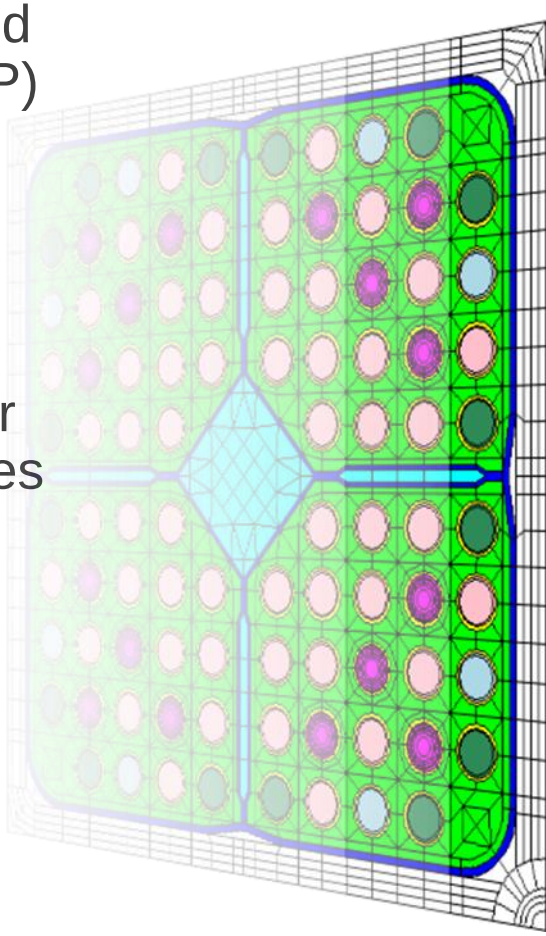
Background

- V&V and qualification of the Westinghouse enhanced BWR simulator code package PHOENIX5/POLCA8 ongoing
  - PHOENIX5 2D deterministic transport code based on Current Coupling Collision Probabilites (CCCP)
    - Unstructured meshing for numerical solution
    - Subgroup resonance treatment method
    - P/C combined with Taylor series expansion of the matrix exponential by uniformization alternatively by solving linearized chains
  - POLCA8 3D steady state nodal core simulator for handling both cartesian and hexagonal geometries
    - Flux solvers based on ANM or AFEN
    - XS model based on microscopic depletion
    - P/C and Taylor series with uniformization
    - Flexible handling of axial heterogenities based on explicit sub-nodes and axial homogenization



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Benchmark Configuration

- 3D single-channel BWR lattice based on OL2 E36 S96O3 design
  - Water diamond and cross replaced with water pins
  - Regular fuel pitch to facilitate Serpent2 pin power edits (`set ppw`)
  - Unchanged nuclear design with PLFRs (12-month cycle)
    - Bottom : 217 – 4.15 w/o U-235, 8x6.00 & 2x3.00 w/o Gd_2O_3
    - Middle : 219 – 4.19 w/o U-235, 8x6.00 & 4x3.00 w/o Gd_2O_3
    - Top : 221 – 4.15 w/o U-235, 8x6.00 & 4x3.00 w/o Gd_2O_3
- Simulated burnup range 0-20 MWd/kgHM

- Boundary conditions
  - Radially : Reflective
  - Axially : Vacuum

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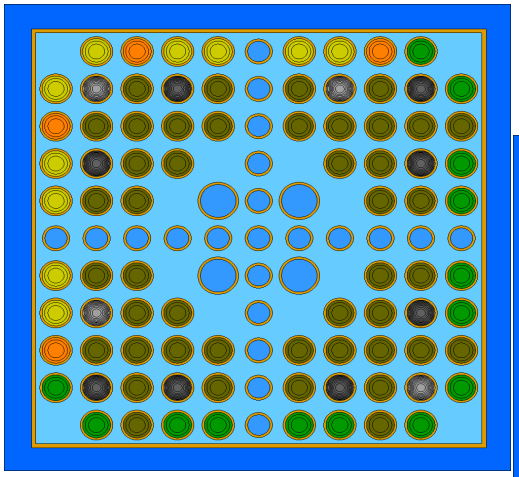
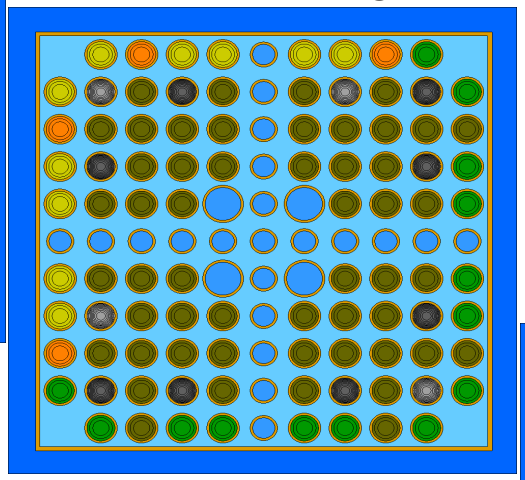
Benchmark Configuration

TOP: 221



MIDDLE: 219



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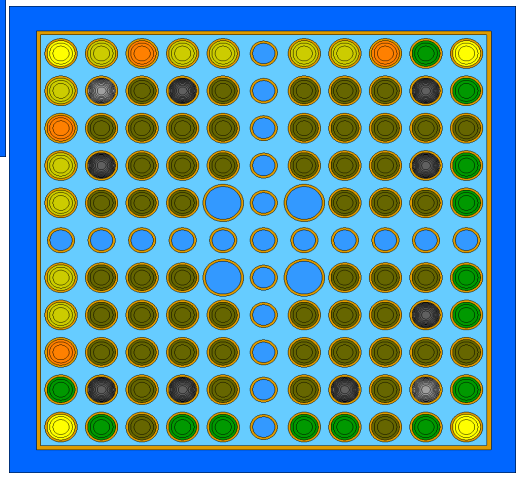

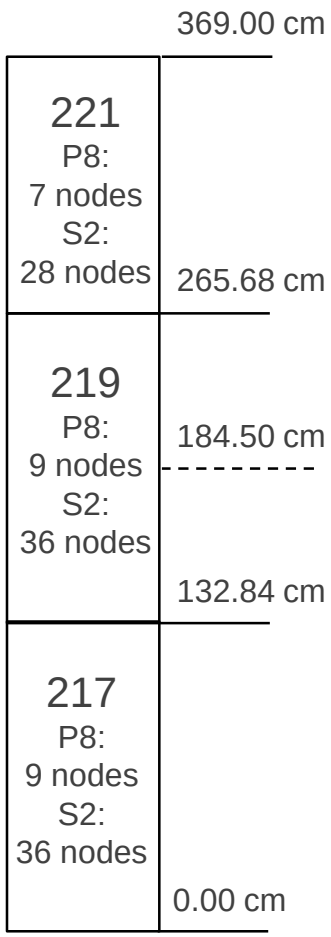

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Benchmark Configuration

- Axial coolant density profile (OL2 BOC38)
- T_m = 559 K
- T_f = 900 K
- Equilibrium xenon

```
% --- Coolant water and axial coolant density profile:

mat cool        -0.73972 moder lwtr 1001
 1001.80c -0.11190083
 8016.80c -0.88809917

ifc "./ifc/coold_type2_BOC.ifc"


2 cool 0
1
1 -6.7385  6.8055 1 -6.8055  6.7385 25 -184.5  184.5
-0.7397200      559.00
-0.7393640      559.00
etc.
```

```
***************
*  DENSACTAV  *          Axial distribution                    Unit = kg/m3    Scale power =  0
***************          ------------------                    ------------    ----------------

 Avg value =  420.29                                  Lin. Rel. Leg. coeff:  -0.66
 Max value =  739.72    Level =  1   Assy = A/01      Qua. Rel. Leg. coeff:   0.26
 Min value =  240.33    Level = 25   Assy = A/01      Cub. Rel. Leg. coeff:   0.00

   Node  Average
                          II---------I---------I---------I---------II
    25    240.33          I            *        :                   I
    24    243.22          I            *        :                   I
    23    247.68          I            *        :                   I
    22    253.75          I             *       :                   I
    21    260.87          I             *       :                   I
    20    269.04          I             *       :                   I
    19    278.20          I              *      :                   I
    18    288.22          I              *      :                   I
    17    299.50          I               *     :                   I
    16    312.38          I                *    :                   I
    15    326.76          I                *    :                   I
    14    342.56          I                 *   :                   I
    13    360.09          I                  *  :                   I
    12    379.48          I                   * :                   I
    11    400.90          I                    *:                   I
    10    425.23          I                     *                   I
     9    454.01          I                     : *                 I
     8    488.94          I                     :   *               I
     7    530.81          I                     :     *             I
     6    579.50          I                     :       *           I
     5    633.77          I                     :         *         I
     4    687.26          I                     :           *       I
     3    725.64          I                     :             *   I
     2    739.36          I                     :             *   I
     1    739.72          I                     :             *   I
                          II---------I---------I---------I---------II
                           0        200       400       600       800
```

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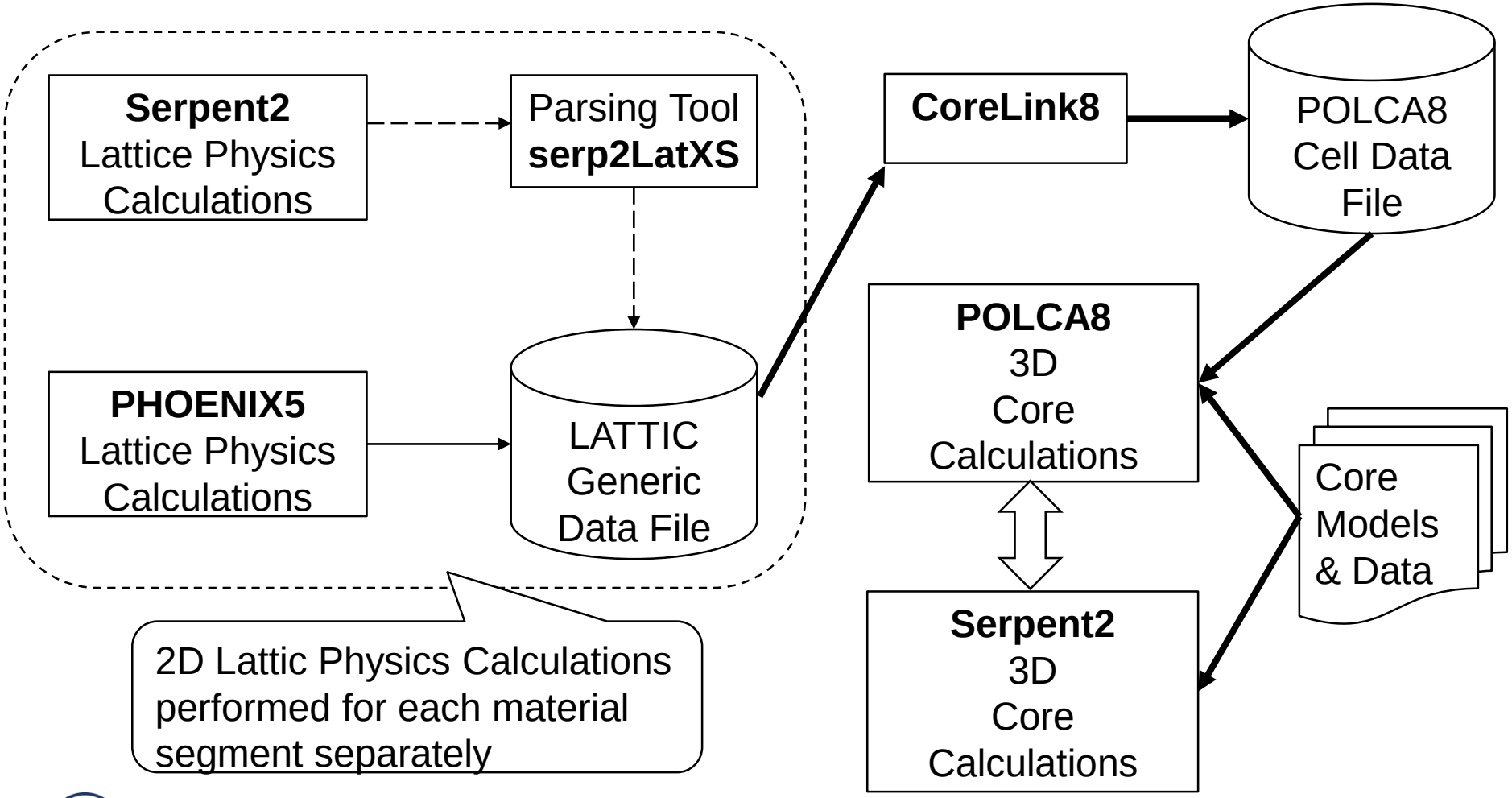
Benchmark Configuration



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2D Lattice Physics Calculations and XS Generation

- Simplified calculation matrix for Serpent2 and PHOENIX5
  - Coolant density histories
    - Void conditions: 00, 30, 60 and 90 %
  - Coolant density branches
    - Burnups: 0, 1, 250, 500, 1000, 2000, 3000, ..., 20000
    - Void conditions: 00, 30, 60 and 90 %
  - Zero xenon branches
    - Same conditions as for coolant density branches
  - CR insertion branches
    - Same conditions as for coolant density branches
    - Not needed in this benchmark
  - CR & zero xenon branches
    - Same conditions as for coolant density branches
    - Not needed in this benchmark
  - No branches for fuel Doppler temperature
  - No critical spectrum search

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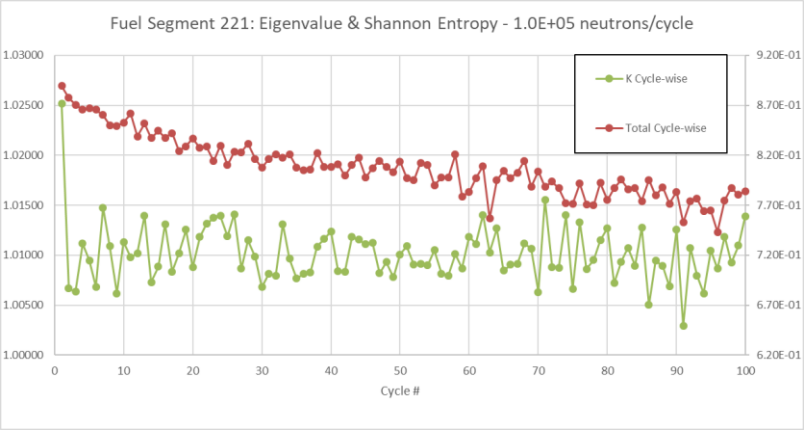
2D Lattice Physics Calculations and XS Generation

- Serpent2 lattice physics
  - 100000 neutrons/cycle x 200 cycles, 100 inactive cycles
  - Statistical uncertainty ≈ 20 pcm or less
  - Running time around few months per history (8 cores/history)
    - Each history and corresponding branches run in parallel
  - DBRC activated – up-scatter effects in resonance treatment
  - Use of unresolved resonance probability table sampling
  - Check of fission source convergence (Shannon entropy)



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Serpent2 3D Reference Calculations

- Important Serpent2 models and options
  - 1000000 neutrons/cycle x 300 cycles
    - At zero burnup 500 inactive cycles
    - Subsequent burnups 200 inactive cycles (`set fsp 1 200`)
  - Statistical uncertainty ≈ 6-7 pcm
  - DBRC activated – up-scatter effects in resonance treatment
    - Increases resonance absorption and lowers reactivity
  - Use of unresolved resonance probability table sampling
  - Depletion with Predictor/Corrector and CRAM (matrix exponential)
    - Burnup step size 250 MWd/t
  - Depletion mesh
    - Axially : 100 nodes with size 3.69 cm
    - Radially : Fuel pins w/o BA – 3 radial rings & 4 sectors
      Fuel pins w/ BA – 10 radial rings & 4 sectors
  - Equilibrium xenon conditions
    - Mesh specification important even for a single power calculation
  - Fixed core coolant density profile and temperatures

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Serpent2 3D Reference Calculations

- Nominal core power set to 10 MW
- Challenges on computing resources (memory and time)
  - The reference calculation required 250 GB of memory
  - The problem run on 24 cores about 3.5 months
    - Intel(R) Xeon(R) CPU E7-8857 v2 @ 3.00GHz, 1200 & 3000 MHz
- Probing calculations to address
  - Fission source convergence
    - Very bottom peaked power distribution
    - Many neutrons need to move starting with a flat distribution
  - Inter-cycle eigenvalue bias
    - Normalization of neutron population between generations
    - Bias proportional to 1/N with N = number of neutrons/cycle
    - Bias not dependent on number of active cycles
  - Very useful paper by Forrest Brown discussing these issues

    "A Review of Best Practices for Monte Carlo Criticality Calculations," ANS 2009 Nuclear Criticality Safety Topical Meeting, Richland, WA, 13-17 September 2009

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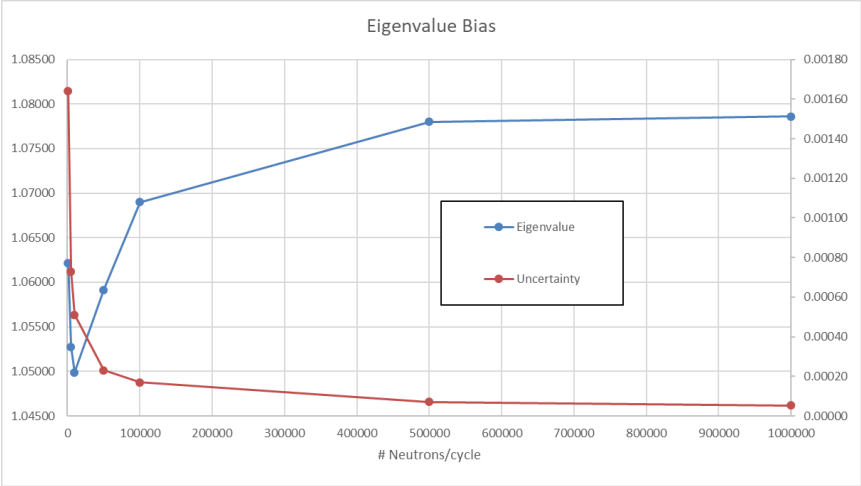
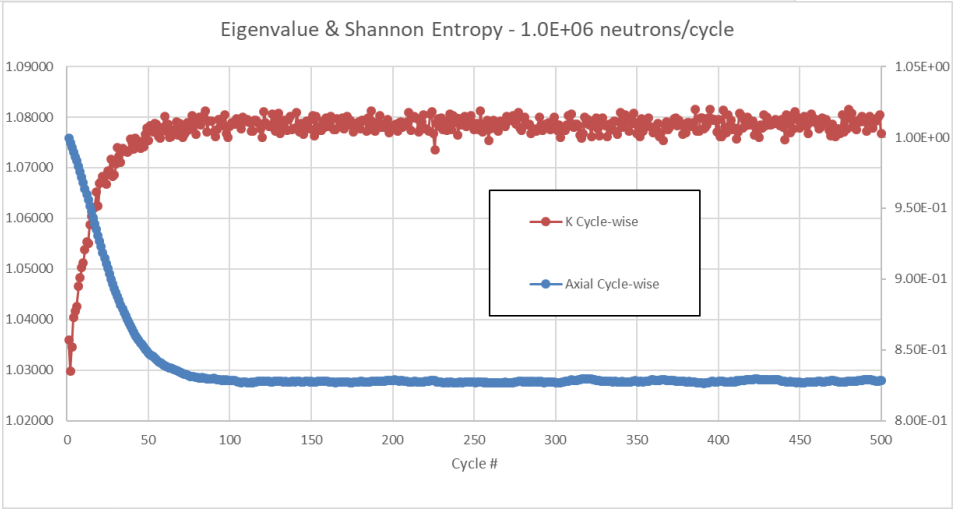
Serpent2 3D Reference Calculations

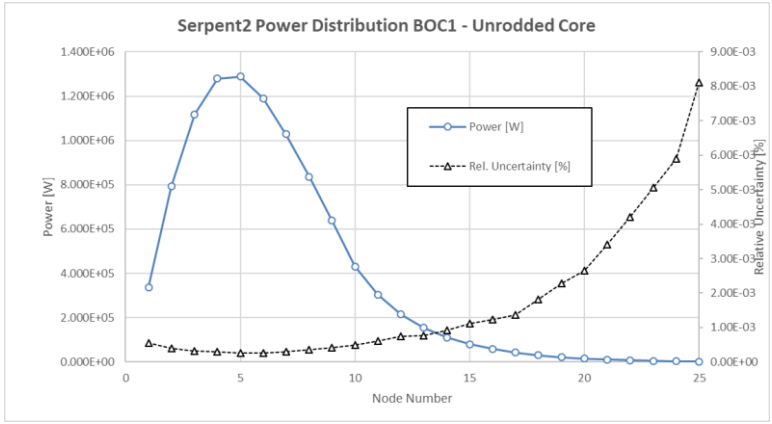


Eigenvalue Bias: 500 inactive cycles

# Cycles w/ 1.0E+06 neutrons	Eigenvalue	Uncertainty	Difference [pcm]
2000	1.07866	0.00003	N/A
1000	1.07868	0.00004	2
500	1.07859	0.00005	-7
250	1.07856	0.00007	-10
125	1.07871	0.00009	5

# Neutrons/cycle w/ 500 cycles	Eigenvalue	Uncertainty	Difference [pcm]
1000000	1.07859	0.00005	N/A
500000	1.07799	0.00007	-60
100000	1.06898	0.00017	-961
50000	1.05912	0.00023	-1947
10000	1.04987	0.00051	-2872
5000	1.05274	0.00073	-2585
1000	1.06215	0.00164	-1644





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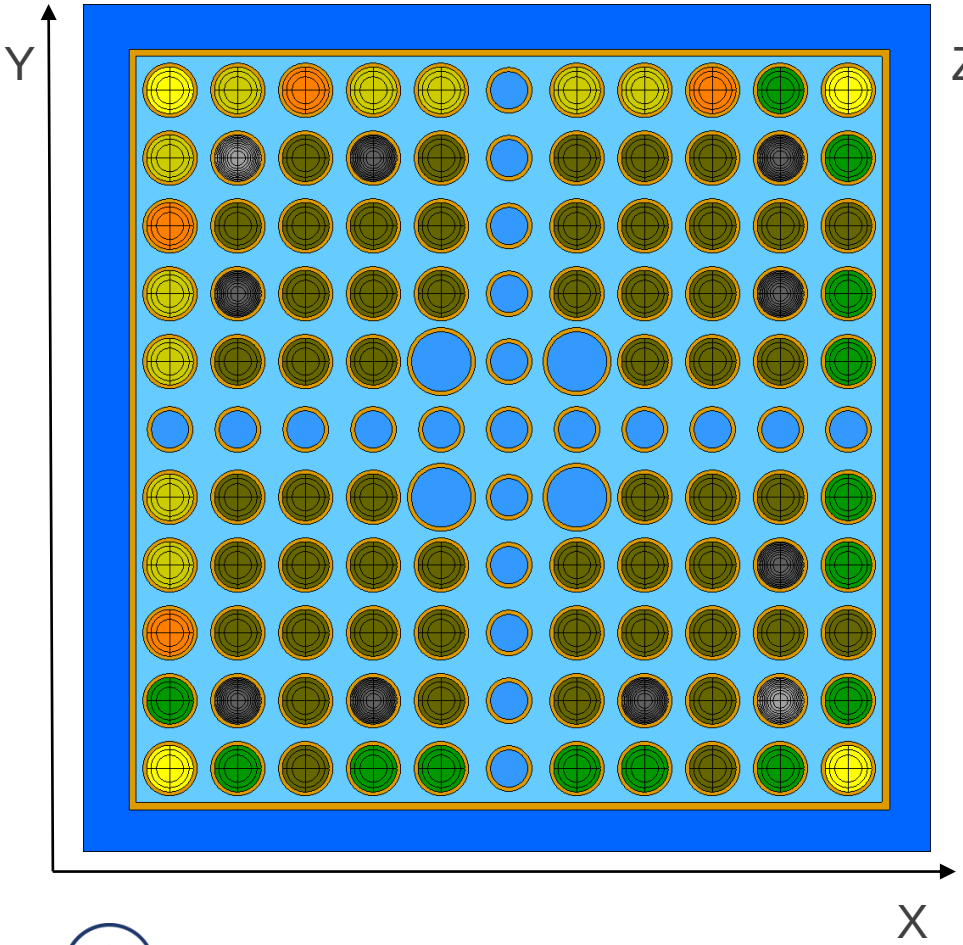
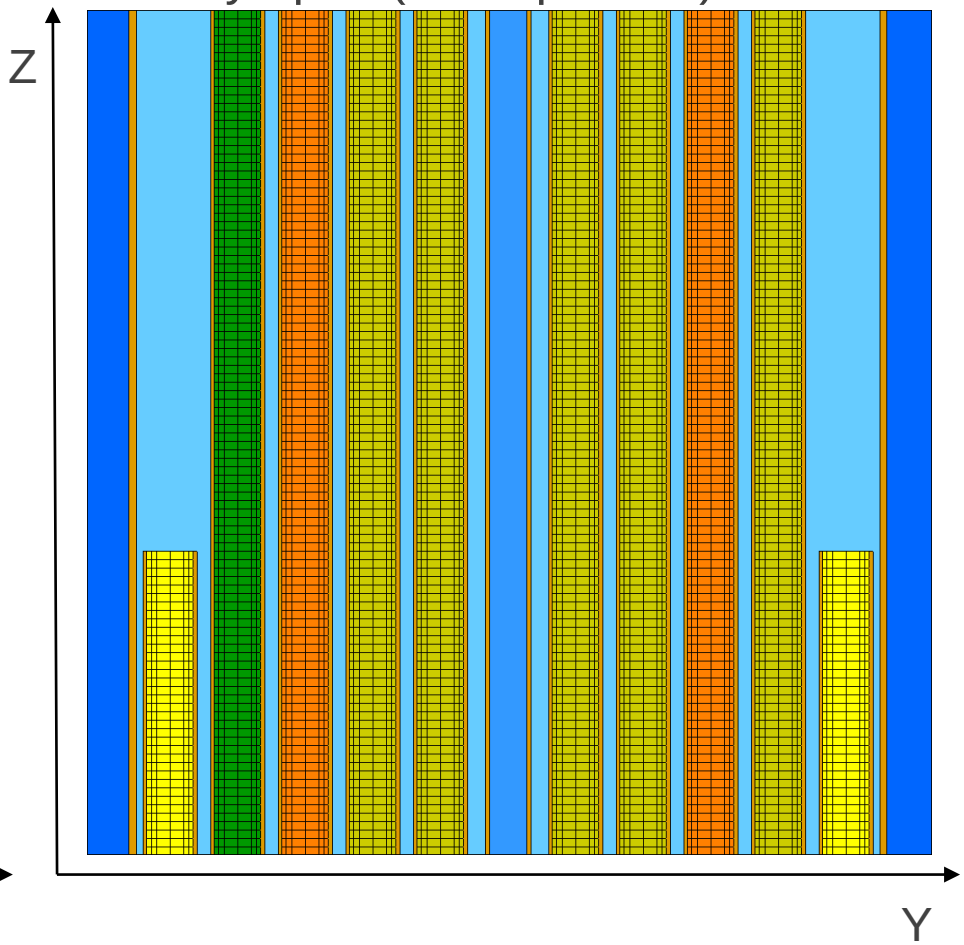
Serpent2 3D Reference Calculations

Radial xy-plot (bottom of core)



Axial yz-plot (outer pin row)



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POLCA8 Calculations

- Important POLCA8 models and options
  - Neutronics based on Analytic Nodal Method (ANM)
  - Depletion with Predictor/Corrector time integration
    - Standard scheme with no corrector step iterations
  - Equilibrium xenon conditions
    - Base xenon NDs computed by the lattice code
    - Xenon coefficients available (xenon spectrum effects)
  - No thermal hydraulics with fixed core axial coolant density profile and fixed temperatures (moderator and fuel)
  - Depletion mesh
    - Axially : 25 nodes with size 14.76 cm (no sub-division of nodes)
    - Radially : 1 node/assembly – assembly pitch 15.375 cm
- Nominal 2x2 homogeneous core power set to 40 MW
  - Edits of results for north-west assembly with power 10 MW

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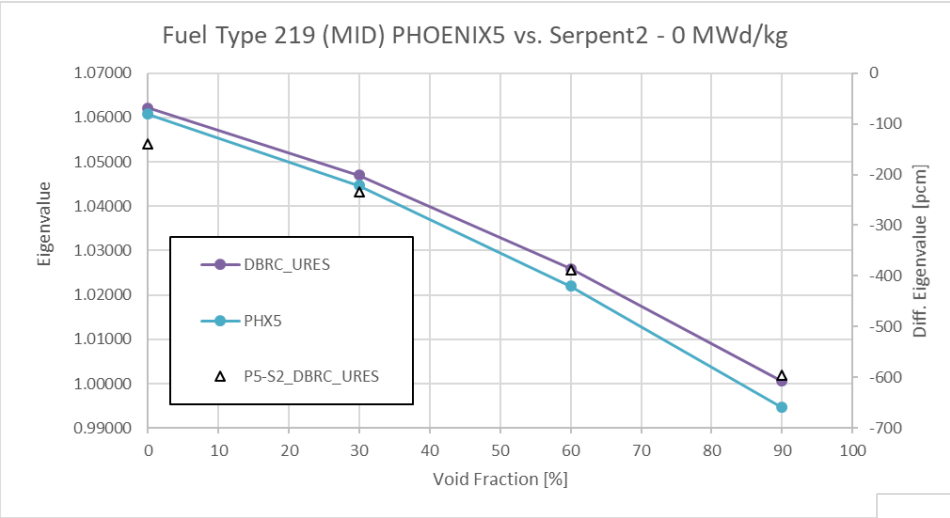
2D Lattice Physics Results – Eigenvalues

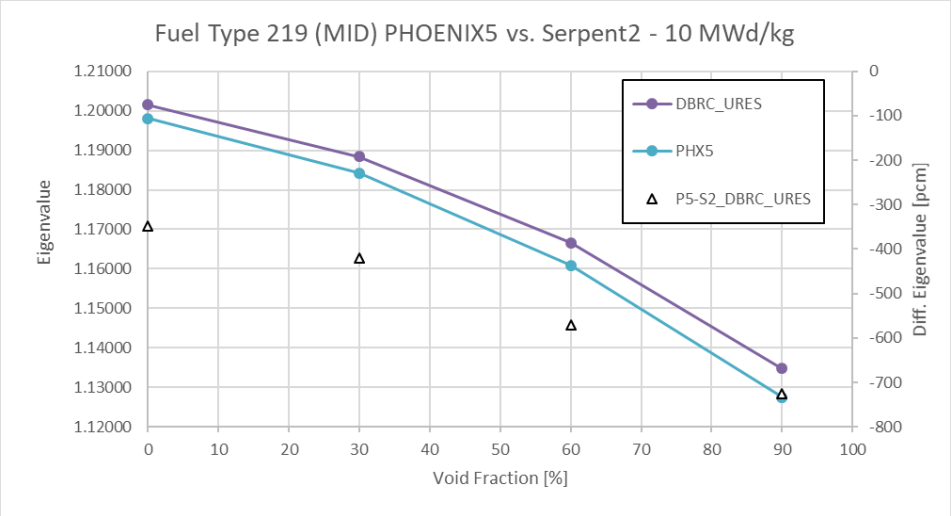


Burnup: 0 MWd/kgHM

Void Fraction [%]	DBRC_URES	PHX5	P5-S2_DBRC_URES
0	1.06211	1.06071	-140
30	1.04695	1.04461	-234
60	1.02587	1.02199	-388
90	1.00059	0.99464	-595
		Max Swing:	455

Burnup: 10 MWd/kgHM

Void Fraction [%]	DBRC_URES	PHX5	P5-S2_DBRC_URES
0	1.20154	1.19805	-349
30	1.18845	1.18425	-420
60	1.16662	1.16092	-570
90	1.13478	1.12752	-726
		Max Swing:	377



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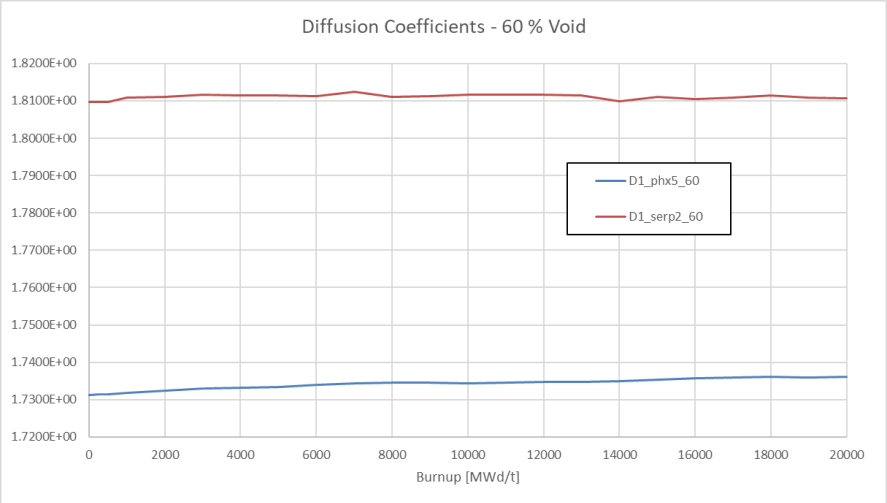
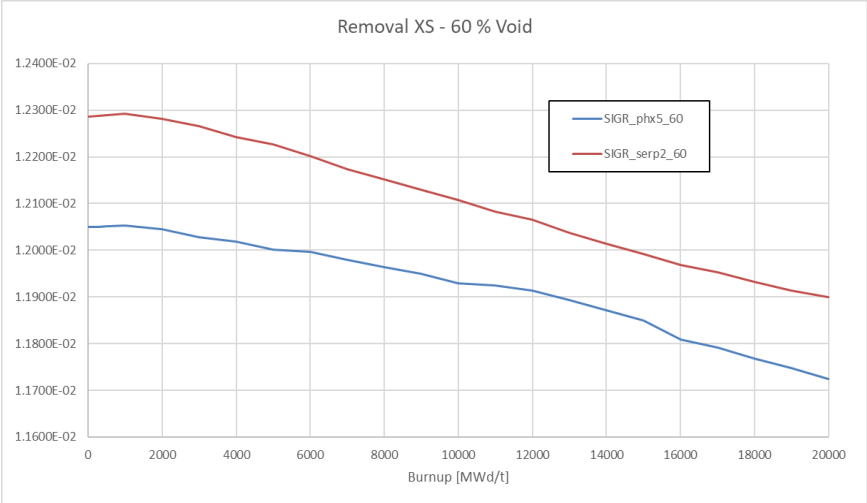
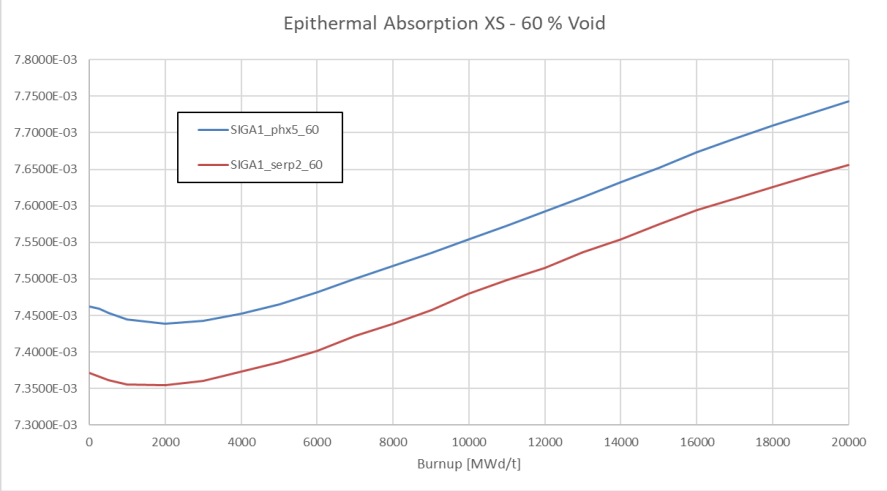
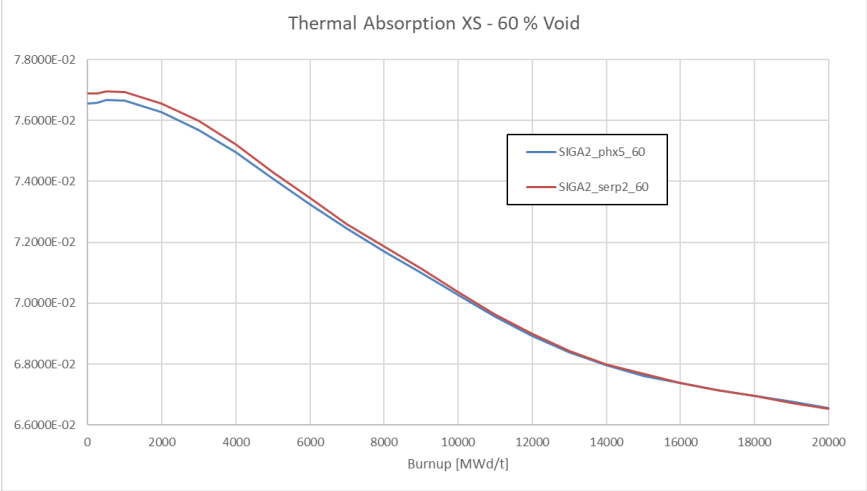
2D Lattice Physics Results – Macroscopic XSs









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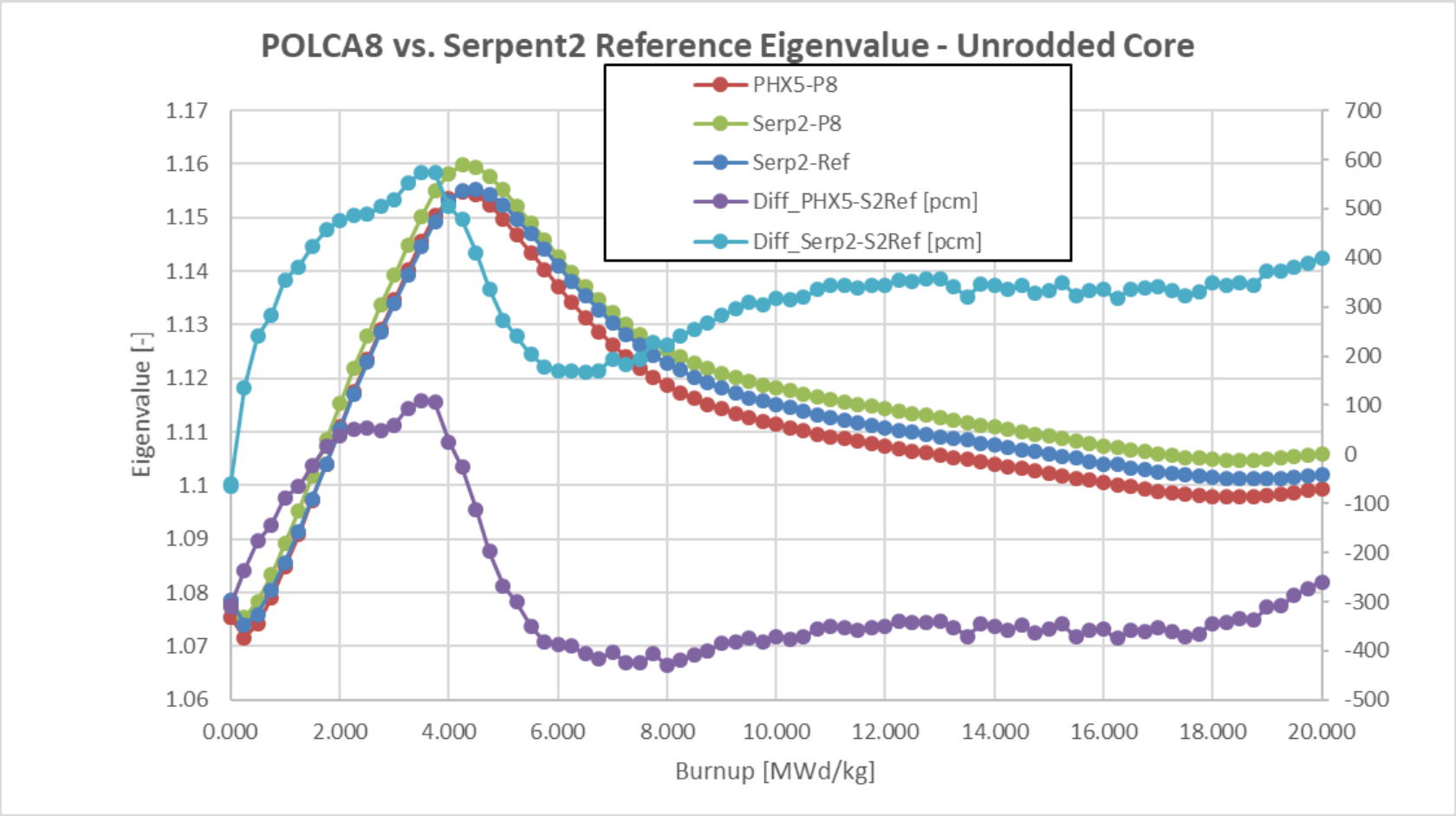
3D Simulation Results – Eigenvalues



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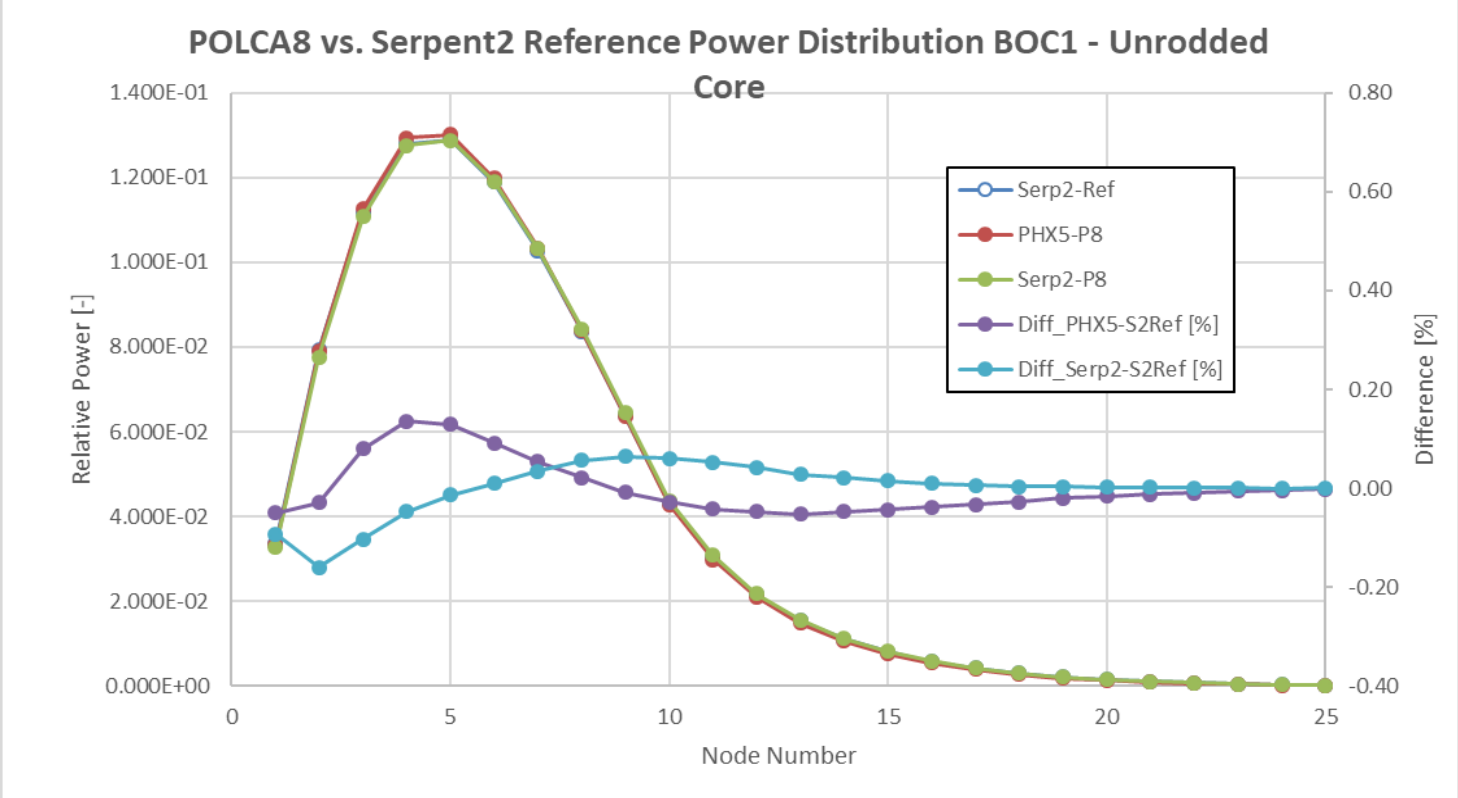
3D Simulation Results – Power Distributions



Core Eigenvalues:								
S2 Reference (+/- 6 pcm)	1.07861	Diff. [pcm]	Base	CR	Xenon	Ax. Leak.	Spat. XS	Fast Leak.
PHOENIX5-POLCA8	1.07551	-310	1.09490	0.00000	-0.00729	-0.01195	-0.00011	-0.00004
Serpent2-POLCA8	1.07802	-59	1.09726	0.00000	-0.00703	-0.01205	-0.00011	-0.00005
Diff. [pcm]	-251		-236	0	-26	10	0	1

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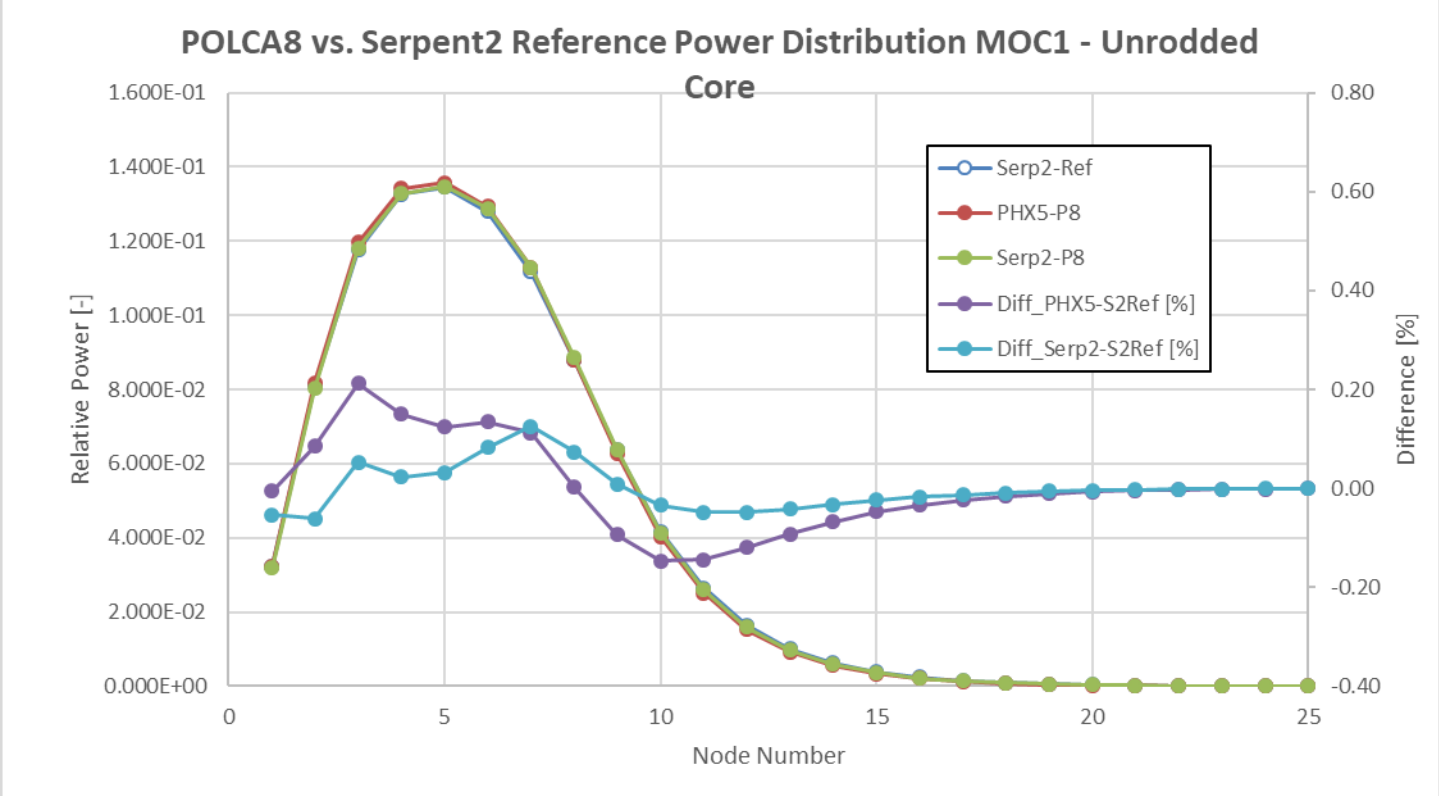
3D Simulation Results – Power Distributions



Core Eigenvalues:										
S2 Reference (+/- 6 pcm)	1.15243	Diff. [pcm]	Base	CR	Xenon	Ax. Leak.	Spat. XS	Fast Leak.	Iso. HN	Iso. FP
PHOENIX5-POLCA8	1.14976	-267	1.17099	0.00000	-0.00994	-0.01144	0.00043	-0.00005	-0.00072	0.00043
Serpent2-POLCA8	1.15516	273	1.17622	0.00000	-0.00986	-0.01150	0.00044	-0.00006	-0.00059	0.00046
Diff. [pcm]	-540		-523	0	-8	6	-1	1	-13	-3

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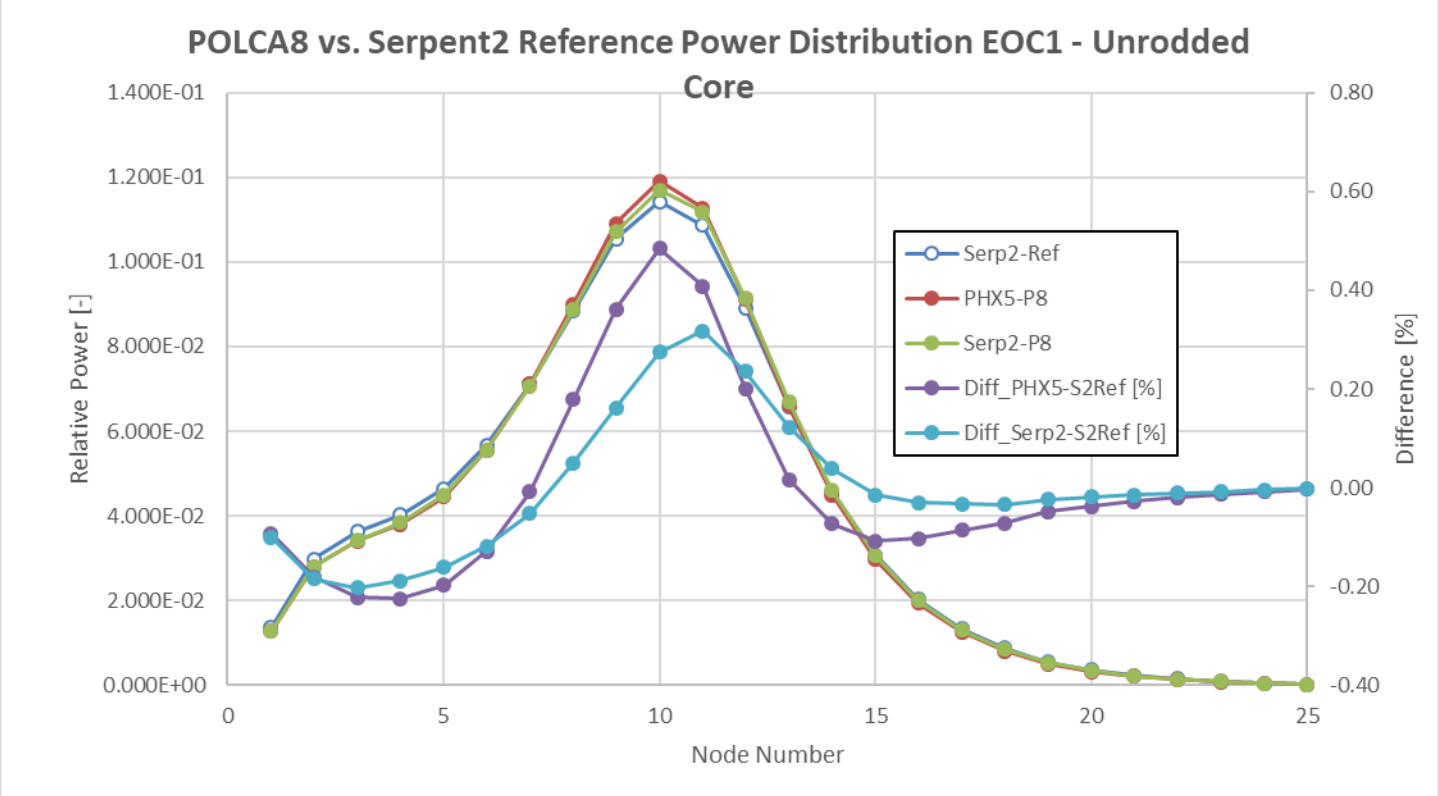
3D Simulation Results – Power Distributions



Core Eigenvalues:										
S2 Reference (+/- 7 pcm)	1.11507	Diff. [pcm]	Base	CR	Xenon	Ax. Leak.	Spat. XS	Fast Leak.	Iso. HN	Iso. FP
PHOENIX5-POLCA8	1.11137	-370	1.12420	0.00000	-0.00810	-0.00451	0.00051	-0.00007	-0.00007	-0.00055
Serpent2-POLCA8	1.11824	317	1.13049	0.00000	-0.00788	-0.00458	0.00051	-0.00007	0.00035	-0.00052
Diff. [pcm]	-687		-629	0	-22	7	0	0	-42	-3

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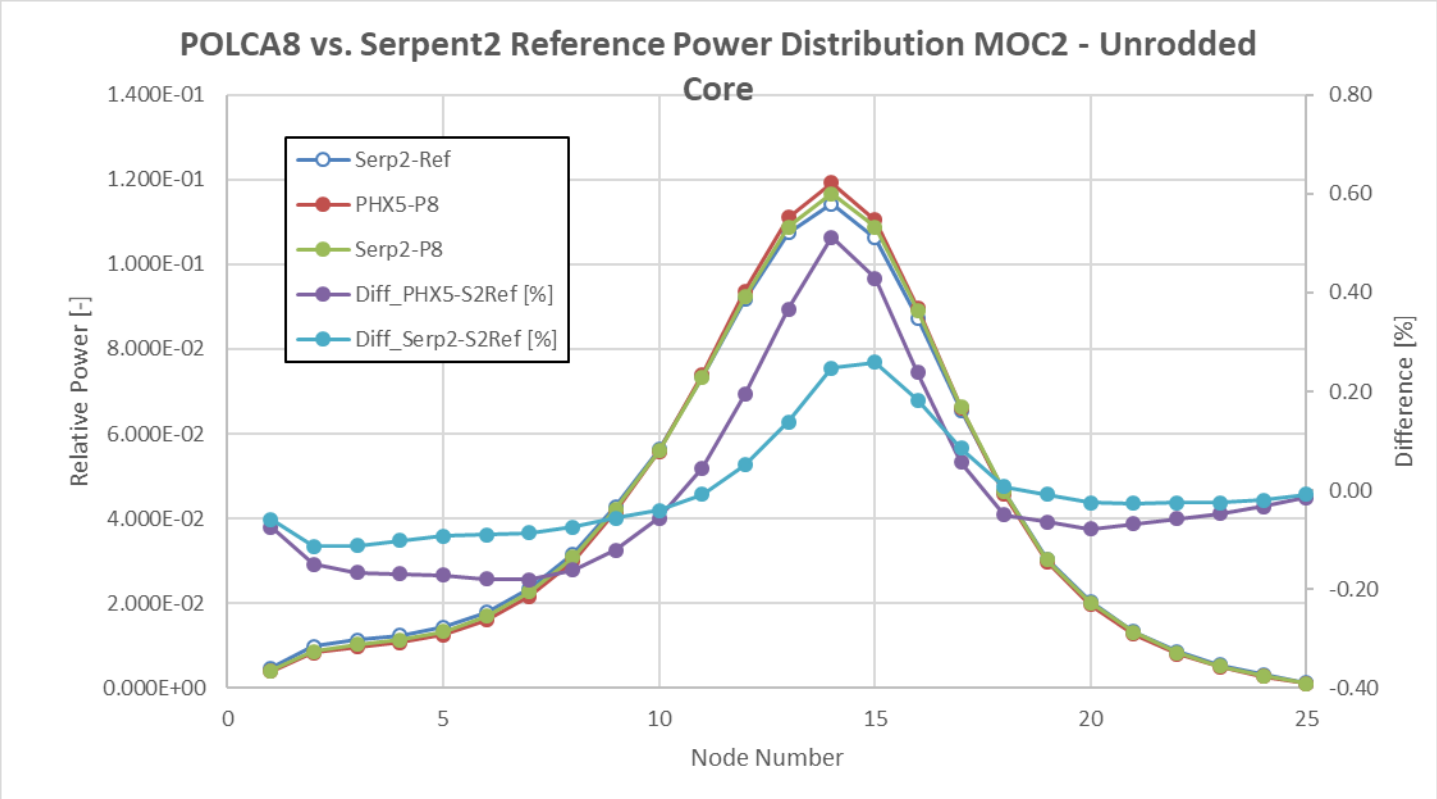
3D Simulation Results – Power Distributions



Core Eigenvalues:										
S2 Reference (+/- 6 pcm)	1.10586	Diff. [pcm]	Base	CR	Xenon	Ax. Leak.	Spat. XS	Fast Leak.	Iso. HN	Iso. FP
PHOENIX5-POLCA8	1.10230	-356	1.11227	0.00000	-0.00791	-0.00215	0.00057	-0.00008	0.00004	-0.00036
Serpent2-POLCA8	1.10920	334	1.11834	0.00000	-0.00771	-0.00230	0.00056	-0.00009	0.00081	-0.00034
Diff. [pcm]	-690		-607	0	-20	15	1	1	-77	-2

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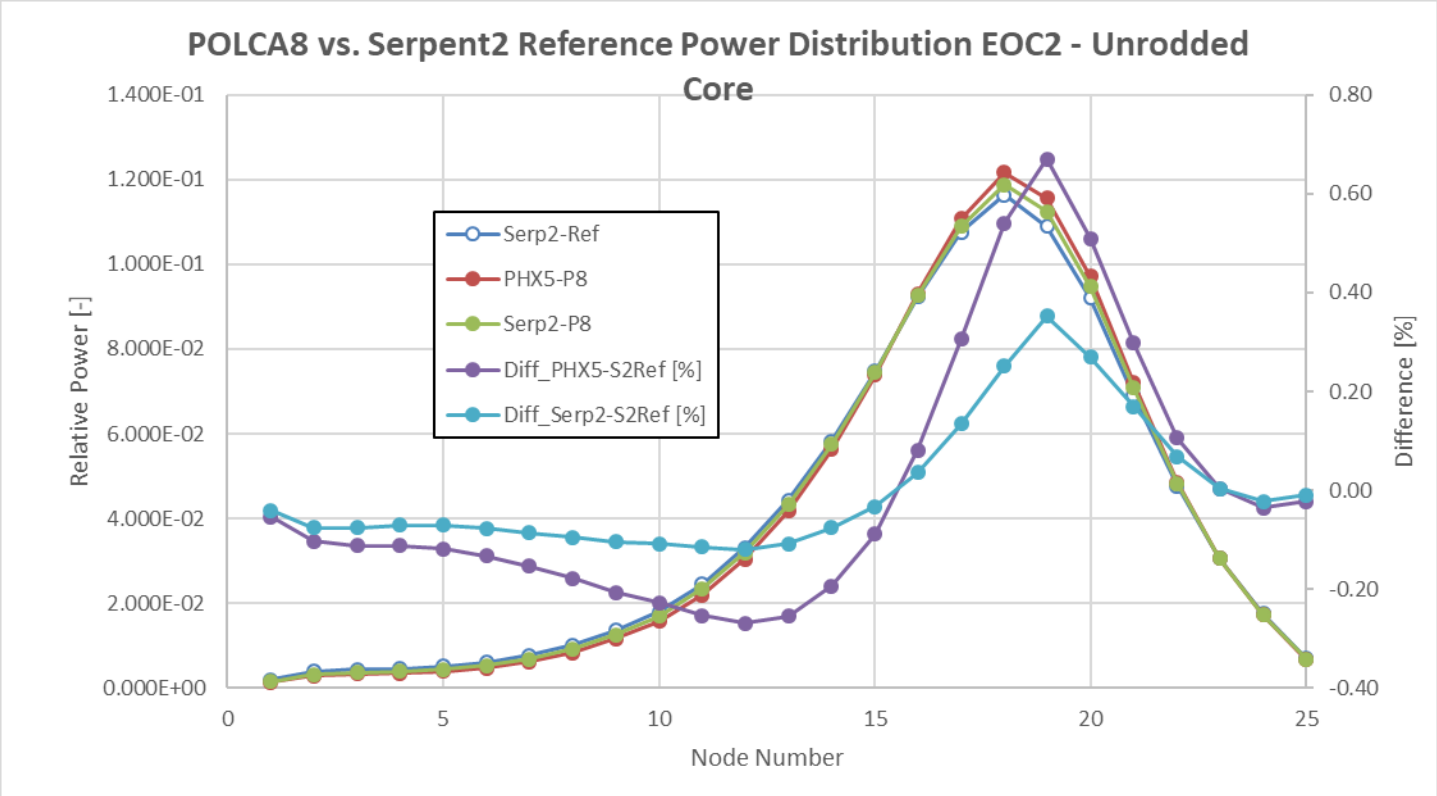
3D Simulation Results – Power Distributions



Core Eigenvalues:										
S2 Reference (+/- 7 pcm)	1.10196	Diff. [pcm]	Base	CR	Xenon	Ax. Leak.	Spat. XS	Fast Leak.	Iso. HN	Iso. FP
PHOENIX5-POLCA8	1.09936	-260	1.11290	0.00000	-0.00835	-0.00520	0.00068	-0.00010	-0.00012	-0.00030
Serpent2-POLCA8	1.10596	400	1.11871	0.00000	-0.00822	-0.00550	0.00067	-0.00010	0.00079	-0.00026
Diff. [pcm]	-660		-581	0	-13	30	1	0	-91	-4

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Summary of Main Observations

- 2D lattice physics results
  - PHOENIX5 underestimates reactivity slightly with ≈ 300 pcm in average compared to Serpent2
    - Level of k-infinity drops with burnup few hundreds of pcm
    - Void dependence of these differences – decreases with burnup
  - PHOENIX5 predicts a somewhat harder spectrum compared to Serpent2
    - Lower SIGR and inherently weaker moderation
    - Higher SIGA1 and inherently stronger resonance absorption
    - Lower D1 and inherently weaker leakage
  - These results have initiated some further investigations in PHOENIX5 to understand these differences
    - Scattering kernel (SIGR)
    - Resonance absorption (SIGA1)
    - Transport correction (D1)

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Summary of Main Observations

- 3D single-assembly core results
  - Overall the reactivity is predicted very well
    - Serpent2/POLCA8 overpredicts slightly the core reactivity
      - POLCA8 microscopic depletion method seems to be insufficient to capture all history effects of this configuration
      - Some contributions from 3D transport effects missing in XSs
        - The effect can be analyzed by generating 3D XSs with Serpent2
    - PHOENIX5/POLCA8 underpredicts slightly the core reactivity
      - Consistent with the 2D results
    - Differences in the eigenvalue level mainly due to different void dependence inherent in base cross sections
    - Same trends with burnup obtained with both code sequences
  - Nodal power distribution very well predicted
    - The power errors at BOC < 0.2 %
    - The power errors increase with burnup but still below ≈ 0.6 %
    - PHOENIX5/POLCA8 seems to predict slightly larger errors

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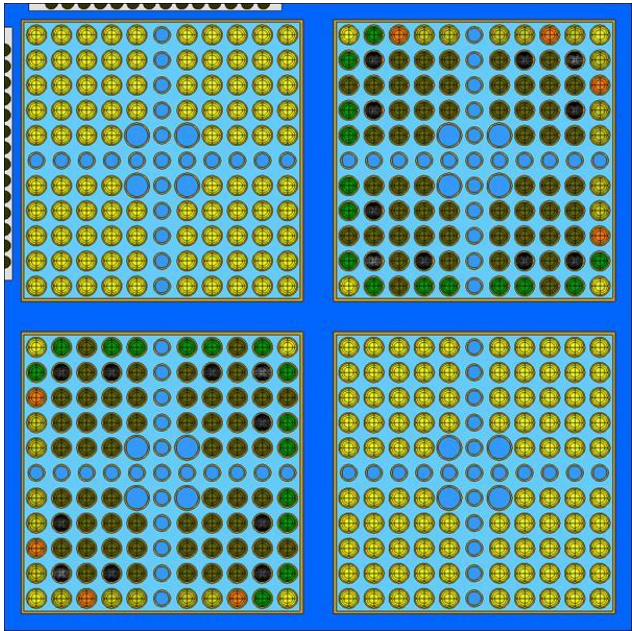
Conclusions and Future Work

- Serpent2 has demonstrated to be an excellent reference tool for benchmarking
  - A significant effort has been invested to develop this framework
  - Necessary for obtaining unambigous comparisons in 3D
  - Easy to make complex geometrical models through universe layers
  - Probing calculations very important to address known challenges in Monte Carlo calculations
  - Very demanding on computer resources (memory and CPU)
- The POLCA8 capability of predicting the core reactivity and power distributions accurately for challenging BWR core conditions was confirmed
- Activities in the near future
  - 3D BWR 2x2 mini-core evaluations of rodded conditions and of the CBH effect
    - M.Sc. thesis project (Mathilde Gaillard, KTH)
    - Planned collaboration with CASL (INL HPC)
    - Results are expected to be obtained during next spring (2021)