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Overview of GENPMAXS/PARCS Capabilities Utilizing SCALE Cross Sections

Andrew Ward
NERS, University of Michigan

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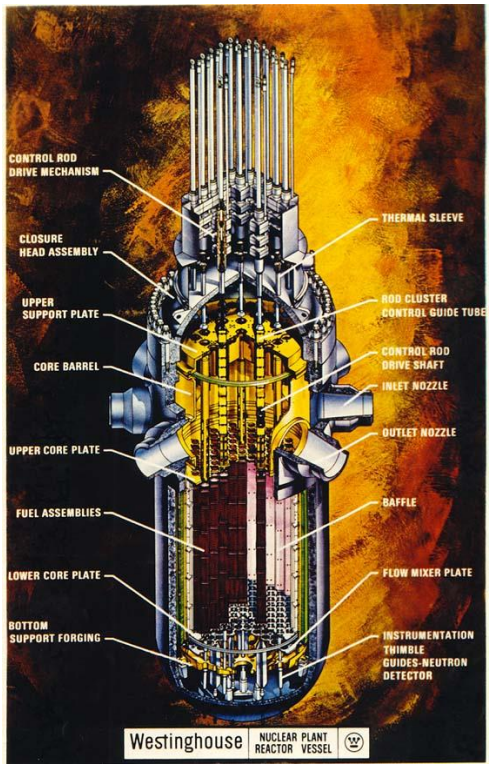
Overview

- Introduction
- Two Step Method / Cross Section Generation
- POLARIS/TRITON-GenPMAXS Interface
- TMI Unit 1 POLARIS-PARCS Results
- WB Unit 2 POLARIS-PARCS Results
- UQ for WB Unit 2 (POLARIS/SAMPLE-PARCS)
- Future Plans

Coupled Neutron / Nuclide Equations



Neutron Transport Equation (Boltzmann)

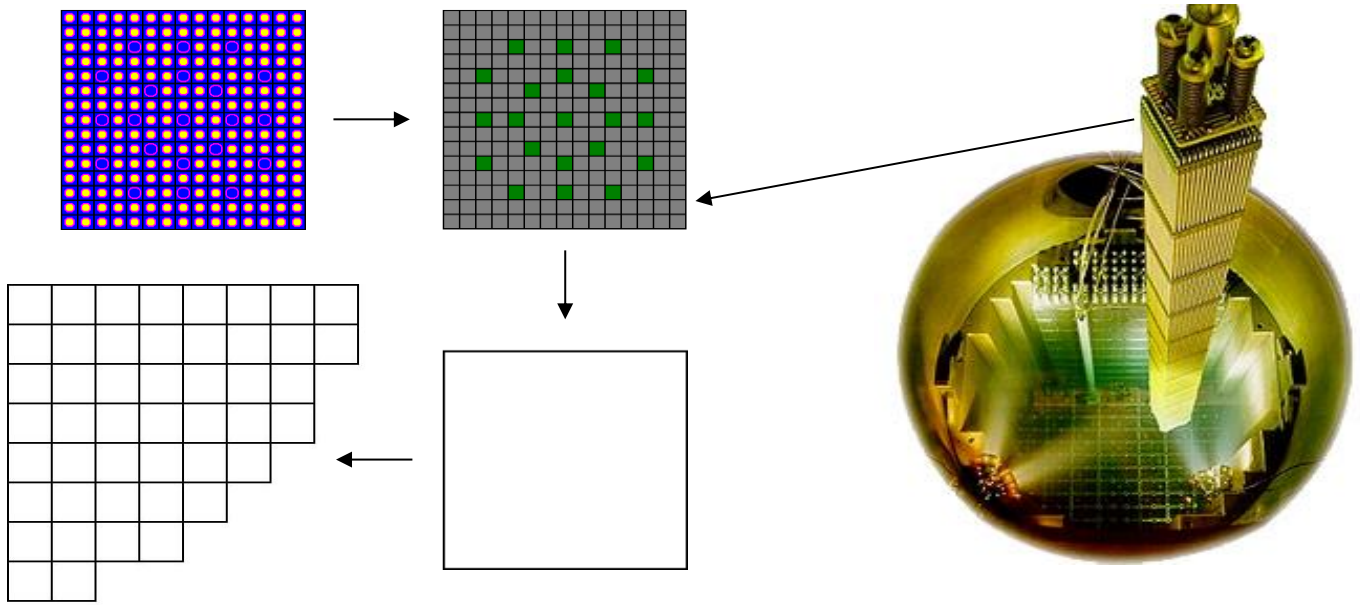
$$\frac{1}{v}\frac{\partial \phi}{\partial t} + \Omega \cdot \nabla \phi(r,E,\Omega,t) + \Sigma_t(r,E)\phi(r,E,\Omega,t) = \frac{1}{4\pi} S_f(r,E,t) + \int_{\Omega'}\int_{E'} \Sigma_s(r,E' \rightarrow E, \Omega' \rightarrow \Omega)\phi(r,E',\Omega',t) dE' d\Omega'$$

Nuclide depletion equation (Bateman)

$$\frac{dN_A(t)}{dt} = -(\sigma_A^a \phi + \lambda_A) N_A(t) + \sigma_C^\gamma \phi N_c(t) + \lambda_B N_B(t)$$

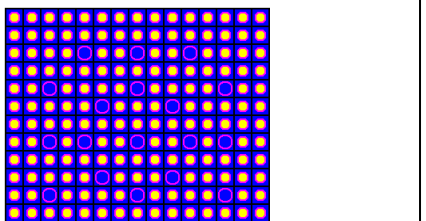
- "2-Step Procedure"
  - Pre-generate homogenized coefficients w/ High Order Solution for fuel assembly → POLARIS Calculation
  - Diffusion Approximation for Core Calculation → PARCS Calculation
- PARCS is the US NRC nodal simulator tool, developed since 1995

$$\frac{1}{v}\frac{\partial \phi}{\partial t} + \Omega \cdot \nabla \phi(r,E,\Omega,t) + \Sigma_t(r,E)\phi(r,E,\Omega,t) = \frac{1}{4\pi} S_f(r,E,t) + \int_{\Omega'}\int_{E'} \Sigma_s(r,E' \to E, \Omega' \to \Omega)\phi(r,E',\Omega',t)dE'\,d\Omega'$$

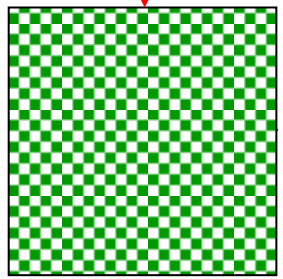


"Two-Step" Solution Method

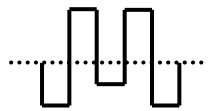
1. Lattice calculation



homogenization



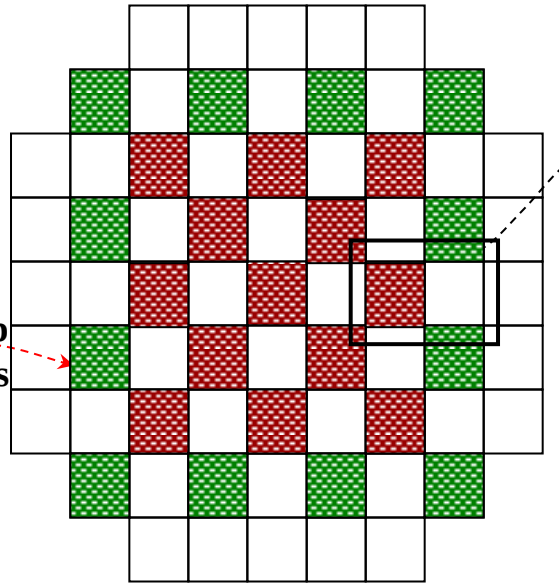
Few Group parameters



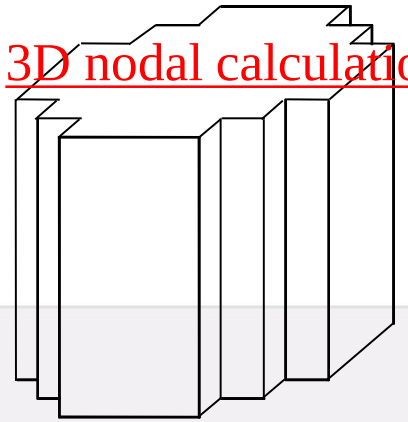
pin factor

$$PF_g(\mathbf{r}) \equiv \frac{\varphi_g(\mathbf{r})}{\bar{\varphi}_g}$$

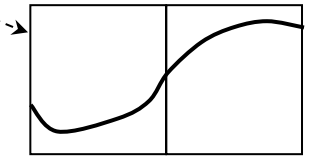
2. Core calculation



3D nodal calculation



Intra-nodal "smooth" flux shape reconstruction



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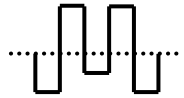
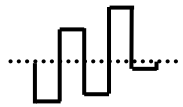
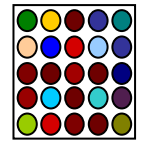




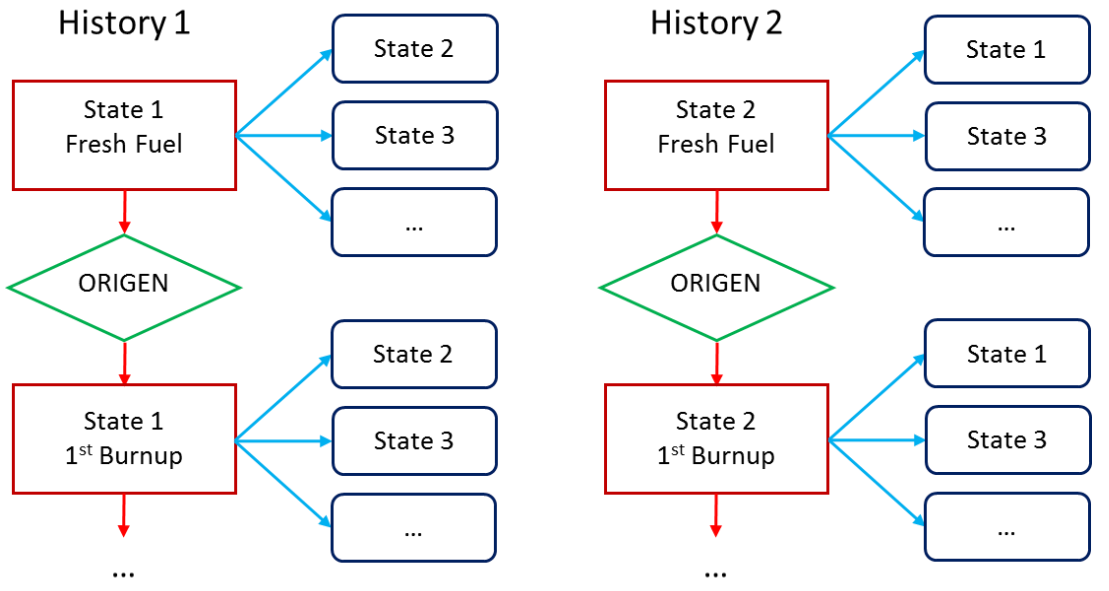


Pin Power

$$\frac{1}{v}\frac{\partial \phi}{\partial t} + \Omega \cdot \nabla \phi(r,E,\Omega,t) + \Sigma_t(r,E)\phi(r,E,\Omega,t) = \frac{1}{4\pi} S_f(r,E,t) + \int\int_{\Omega' E'} \Sigma_s(r,E' \to E, \Omega' \to \Omega)\phi(r,E',\Omega',t)dE'd\Omega'$$

POLARIS/TRITON-PARCS XS Generation Method

- Execute N_h (history) parallel runs with a common set of parameterized state conditions (branches) with burnup
- History cases (H_h) and branches depend on reactor type and simulation space (depletion, transient)



POLARIS/TRITON-GenPMAXS Interface (1/2)

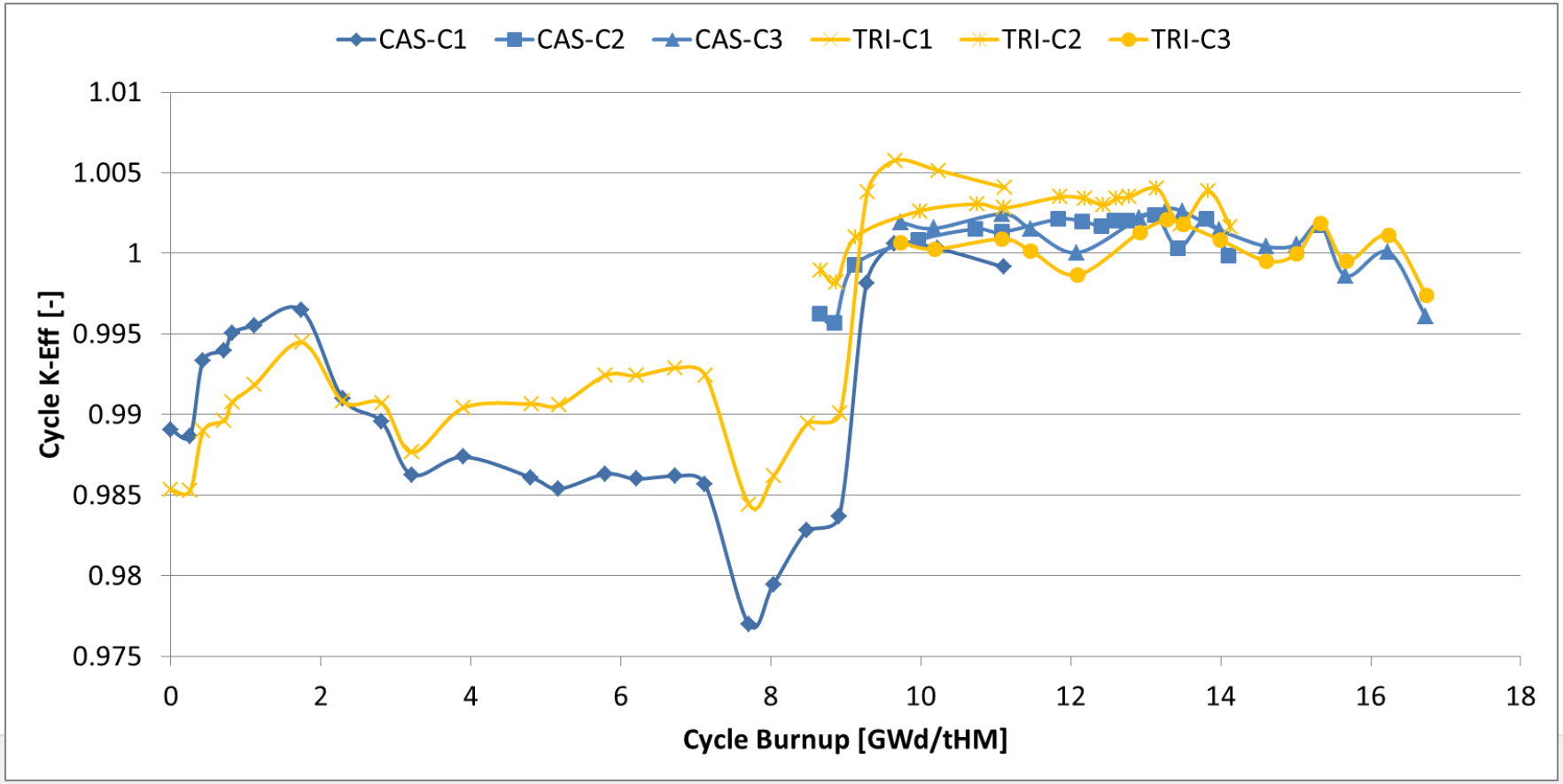
- GenPMAXS: A software tool to read, combine, test, and format raw transport XS data into the the PMAXS format
- POLARIS, TRITON, HELIOS, CASMO, SERPENT, and other codes are supported

- Combine histories into single assembly library
- Calculate required library XS derivatives
- Perform 1D flux calculation for discontinuity factors
- Test transport XS for accuracy and convergence

Experience with TRITON (2005-present)

- Direct experience with LWR depletion
  - BWR: Peach Bottom, Hatch
  - PWR: BEAVRS (Benchmark on physical data)
- Other PARCS users
  - PHWR: CANDU and Atucha (Argentina)
  - Graphite: Prismatic / VHTR
- NRC Staff
  - Some time-dependent accident an analyses

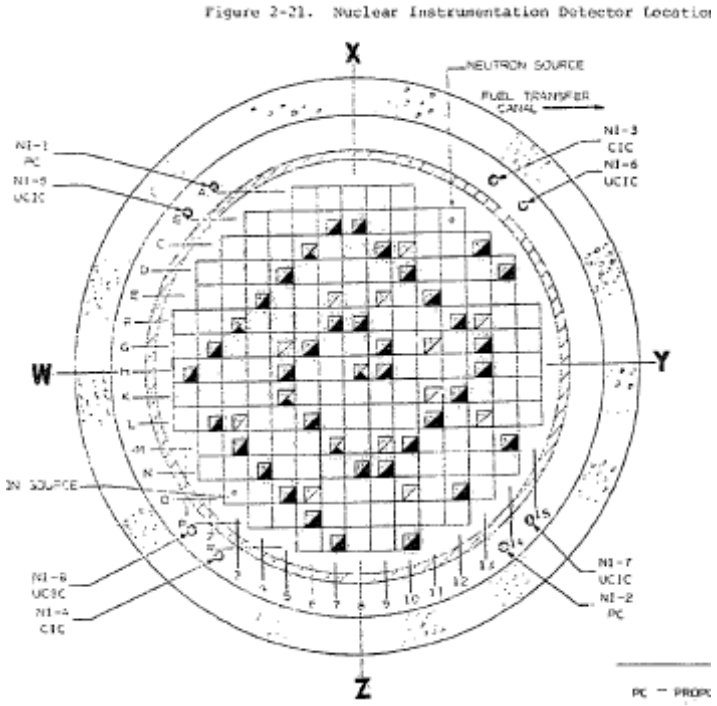
Peach Bottom Depletion (TRITON/PARCS)



- Cross Sections
  - CASMO-4
  - TRITON
- Good agreement after Cyc 1
- ±500 pcm desirable

TMI Unit 1

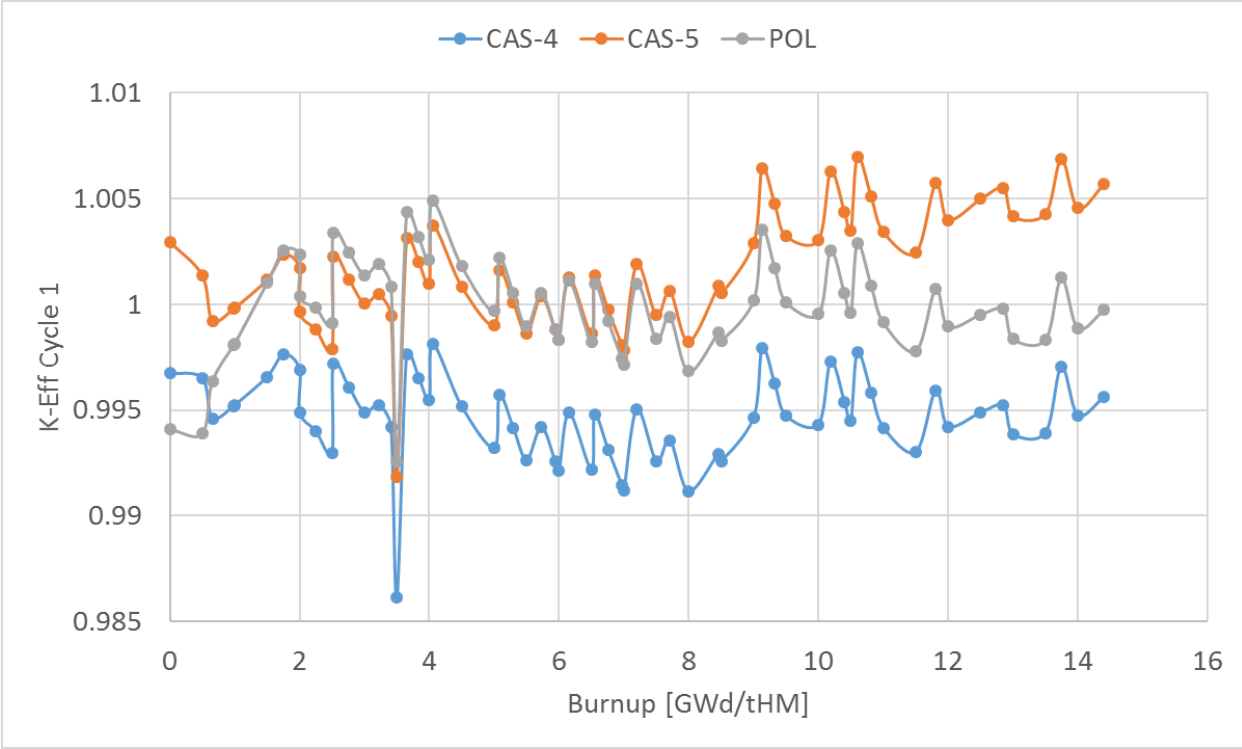
- B&W Plant Design
- 2568 MWt, 560 Assemblies
- Startup April 1974 (FP Sep 74)
- Core follow data for cycles: 1-2



TMI Unit 1 POLARIS-PARCS

- POLARIS-PARCS calculation
  - Compared to CASMO-4,5
- Cycle 1 data well verified
- Generally good agreement with eachother

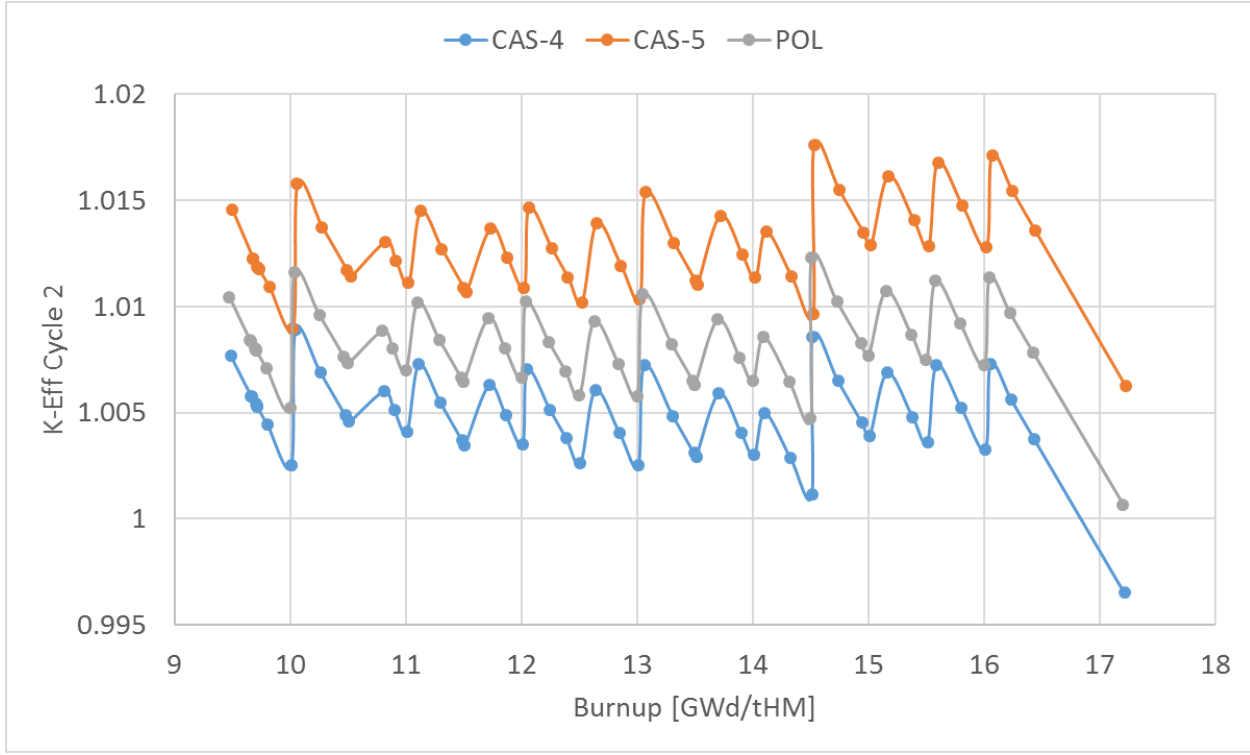
*Note: model was under development for this calc



TMI Unit 1 POLARIS-PARCS

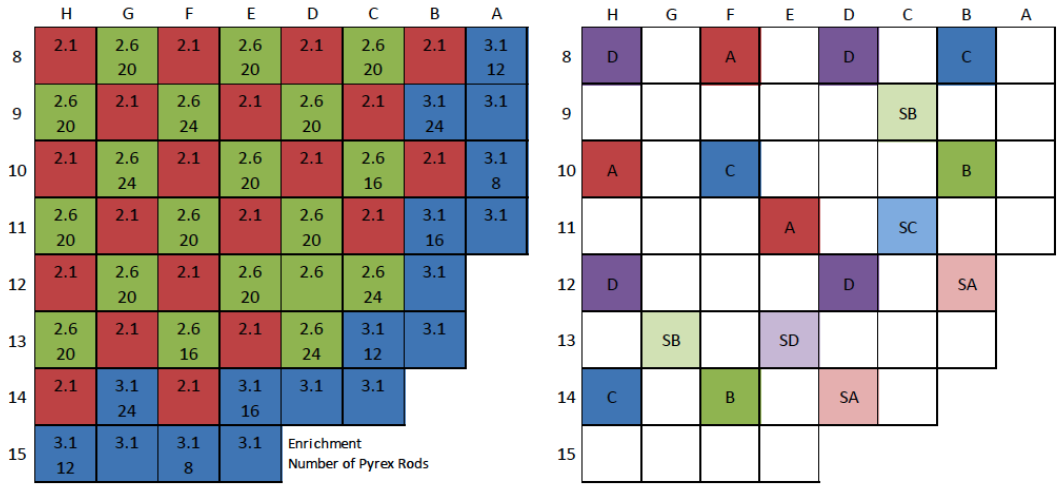
- POLARIS-PARCS calculation
  - Compared to CASMO-4,5
- Cycle 2 poor quality data
- Generally good agreement with eachother

*Note: model was under development for this calc



Watts Bar Unit 2 POLARIS-PARCS

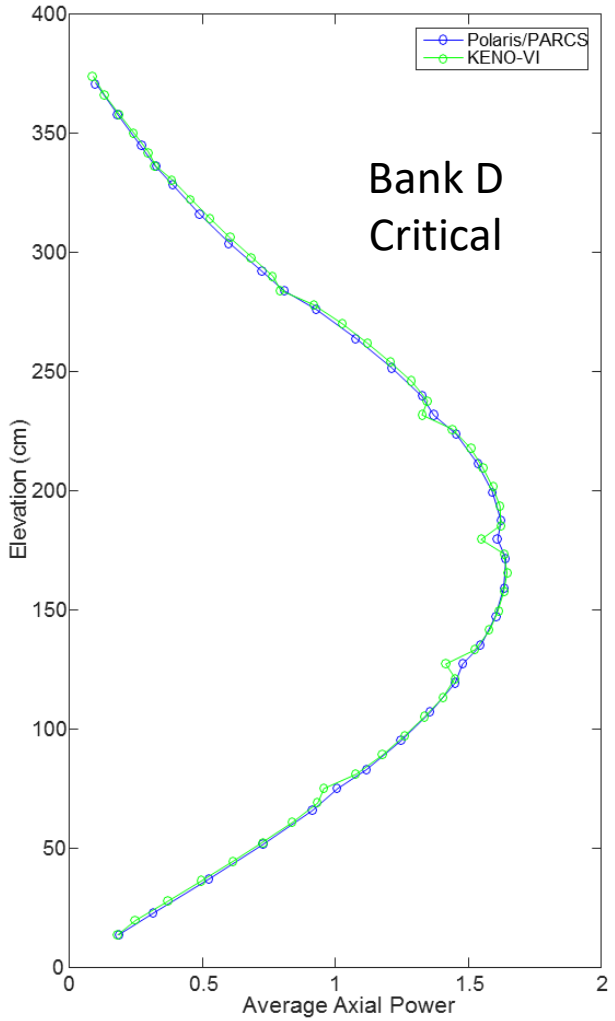
- Westinghouse PWR
- 193 Fuel Bundles, 3411 MWt
- Full Power, October 2016
- Core follow data for cycles: 1-9



Watts Bar Cold Critical Comparison

- Reference results generated with SCALE-KENO
- Very good agreement

Case	Reference k-eff*	POLARIS/PARCS k-eff	Δk pcm
Bank D @ 167 Steps (1285 ppm boron)	0.99989	0.99826	-163
ARO (1290 ppm boron)	1.00032	0.99919	-113



Watts Bar Cold Critical Comparison

- Bank D Criticals
  - D @ 167 steps
  - 1285 ppm Boron
- POLARIS-PARCS
  - RMS Relative Error 1.2%

KENO

	H	G	F	E	D	C
8	0.9487					
9	0.9193	0.9973				
10	1.0181	0.9083	1.0648			
11	0.9850	1.0819	1.0412	1.1615		
12	1.0647	1.0471	1.1746	1.0850	1.2368	
13	1.0480	1.1619	1.1520	1.1508	0.8969	0.9126
14	1.0841	1.0652	1.1039	1.0496	0.9452	0.6296
15	0.7931	0.9071	0.8046	0.6590		

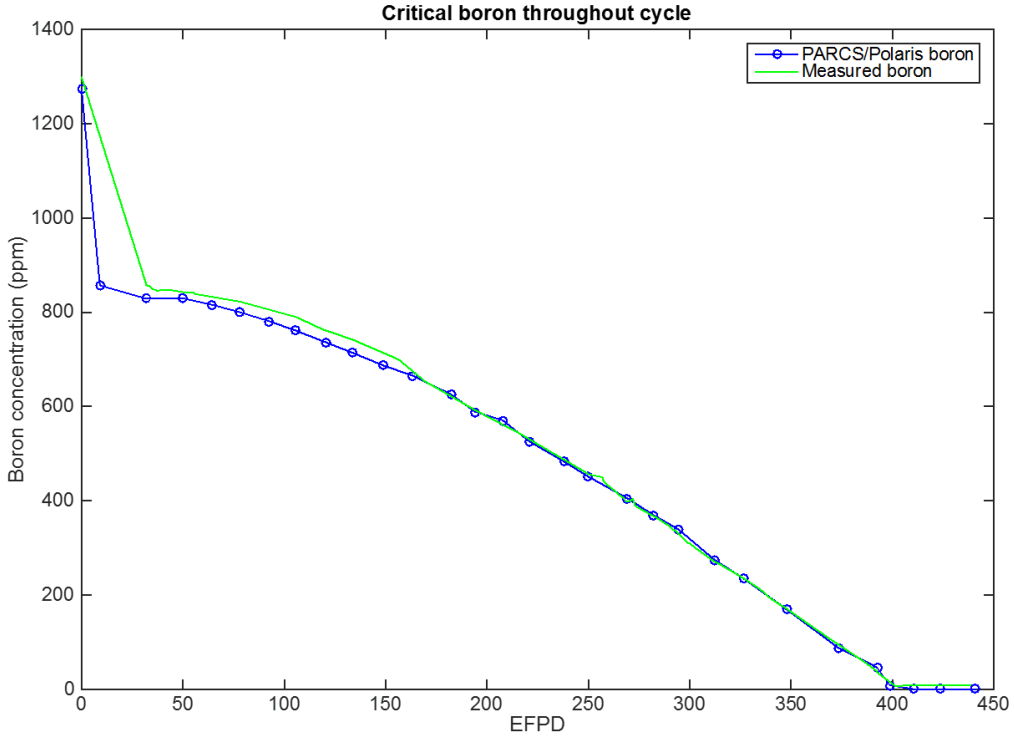
Max: 1.2368 Avg: 1.0000

POLARIS-PARCS

0.9659 (1.81%)					
0.9300 (1.16%)	1.0174 (2.02%)				
1.0378 (1.92%)	0.914 (0.63%)	1.0833 (1.74%)			
0.9919 (0.70%)	1.0991 (1.59%)	1.0475 (0.61%)	1.1758 (1.23%)		
1.0740 (0.87%)	1.0502 (0.30%)	1.1874 (1.09%)	1.0856 (0.06%)	1.2319 (-0.40%)	
1.0456 (-0.23%)	1.1693 (0.64%)	1.1503 (-0.15%)	1.1554 (0.40%)	0.8934 (-0.39%)	0.9066 (-0.66%)
1.0859 (0.17%)	1.0513 (-1.30%)	1.1037 (-0.02%)	1.0380 (-1.11%)	0.9298 (-1.63%)	0.6170 (-2.00%)
0.7827 (-1.31%)	0.8917 (-1.70%)	0.7931 (-1.43%)	0.6461 (-1.96%)		

Watts Bar Cycle 1 Depletion

- Good agreement across the cycle
- No boron measurement at ~10 EFPD



POLARIS/SAMPLER UQ in PARCS

Application to POALRIS-PARCS

- Apply the XS uncertainty quantification to WB2 depletion calculation
- Generate ~100 perturbed XS libraries for each fuel material
- ~100 distinct PMAXS libraries per fuel type; each set of PMAXS files have correlated perturbations

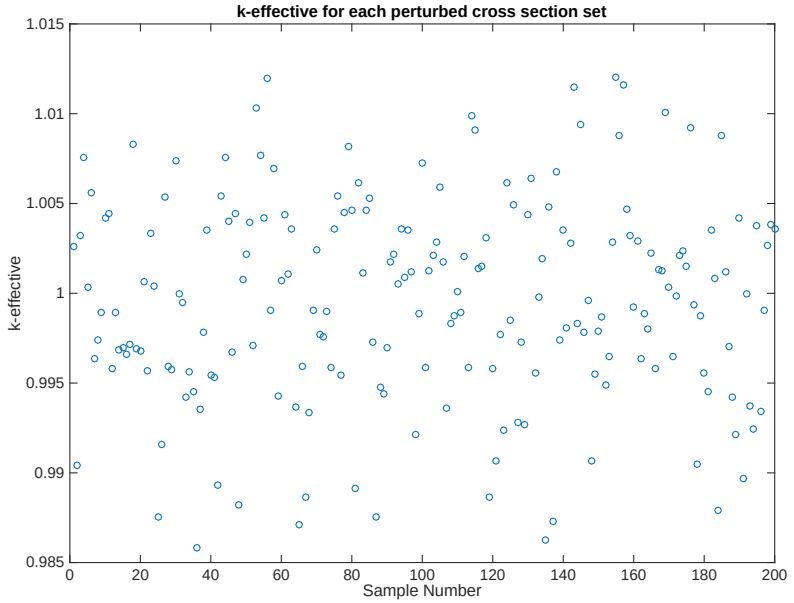
Essence of SAMPLER Sequence

- Random values for the input multigroup cross sections are determined by using the XSUSA program to sample uncertainty data provided in the SCALE covariance library.
- Using these samples, Sampler computes perturbed self-shielded cross sections and propagates the perturbed nuclear data through any specified SCALE analysis sequence including those for criticality safety, lattice physics with depletion, and shielding calculations.

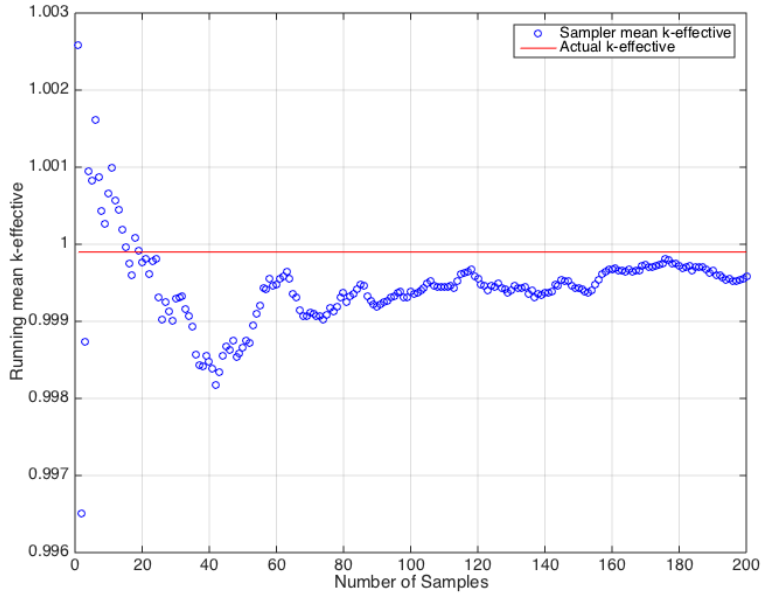
UQ Results, WB2 HZP Critical Core

- Sampler running mean k-eff for HZP critical core vs. number of samples
- Average k-eff vs. num samples plotted below (red line is KENO k-eff)
- 200 samples generated using Sampler-Polaris module
- Perturbed cross sections used in PARCS nodal calculation

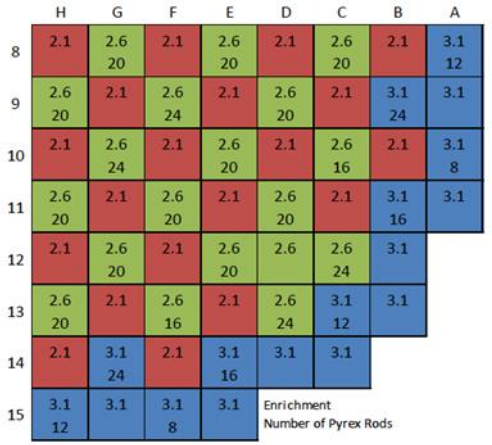
Std. Dev. of k-eff = 565 pcm



Running mean k-eff vs No. Samples



PARCS Radial Power Uncertainty



KENO

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15	0.7931	0.9071	0.8046	0.6590		

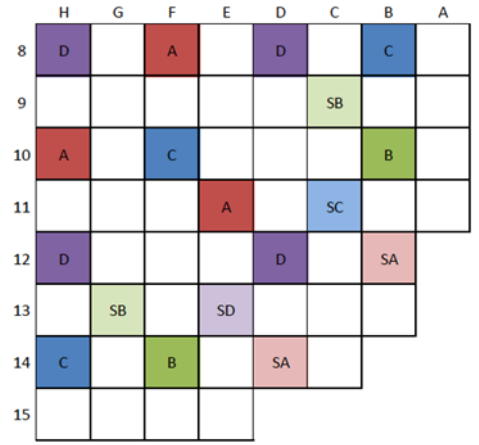
Max: 1.2368 Avg: 1.0000

POLARIS-PARCS

3.72					
3.69	3.45				
3.13	3.13	2.46			
2.45	2.17	1.80	1.01		
1.37	1.29	0.74	0.28	0.72	
0.34	0.12	0.31	0.83	1.21	2.11
1.00	1.08	1.50	1.86	2.37	2.64
1.81	2.16	2.27	2.41		

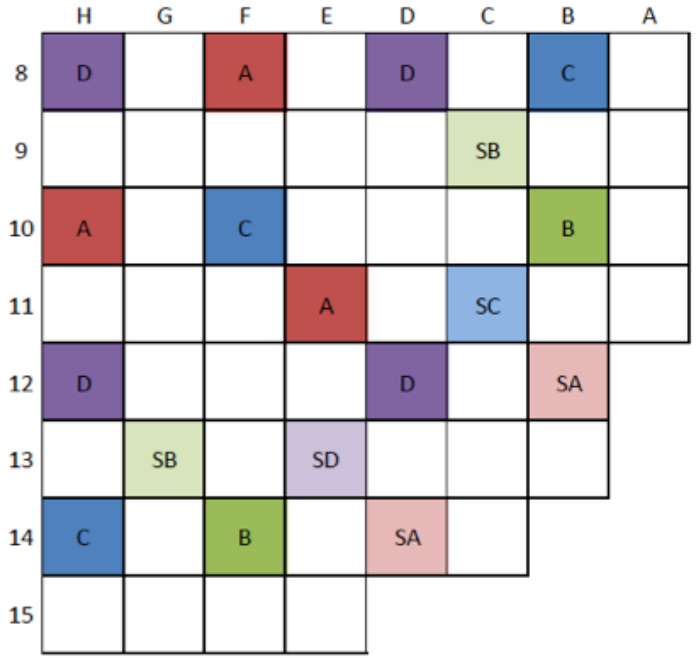
Non BP Assemblies

RMS: 2.05%

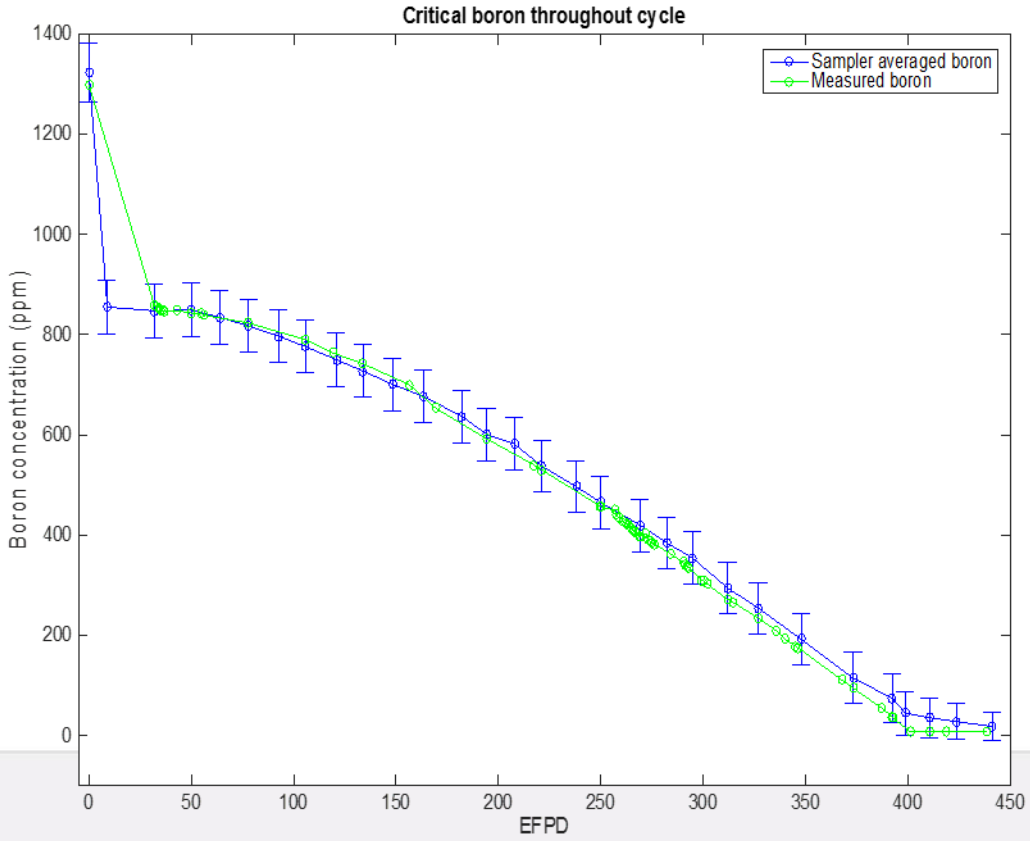


Sampler/Polaris/PARCS: Control Rod Bank Worth Uncertainty

Case	Meas. Worth	Avg. Polaris/ PARCS Worth	Absolute std (pcm)	XSEC Uncertainty (%)
Bank D	1342	1406	26	1.85%
Bank C	951	981	26	2.65%
Bank B	879	871	22	2.53%
Bank A	843	909	44	4.84%
Bank SD	480	464	4	0.86%
Bank SC	480	464	4	0.86%
Bank SB	1056	1057	9	0.85%
Bank SA	435	463	16	3.46%
RMS	-	-	-	

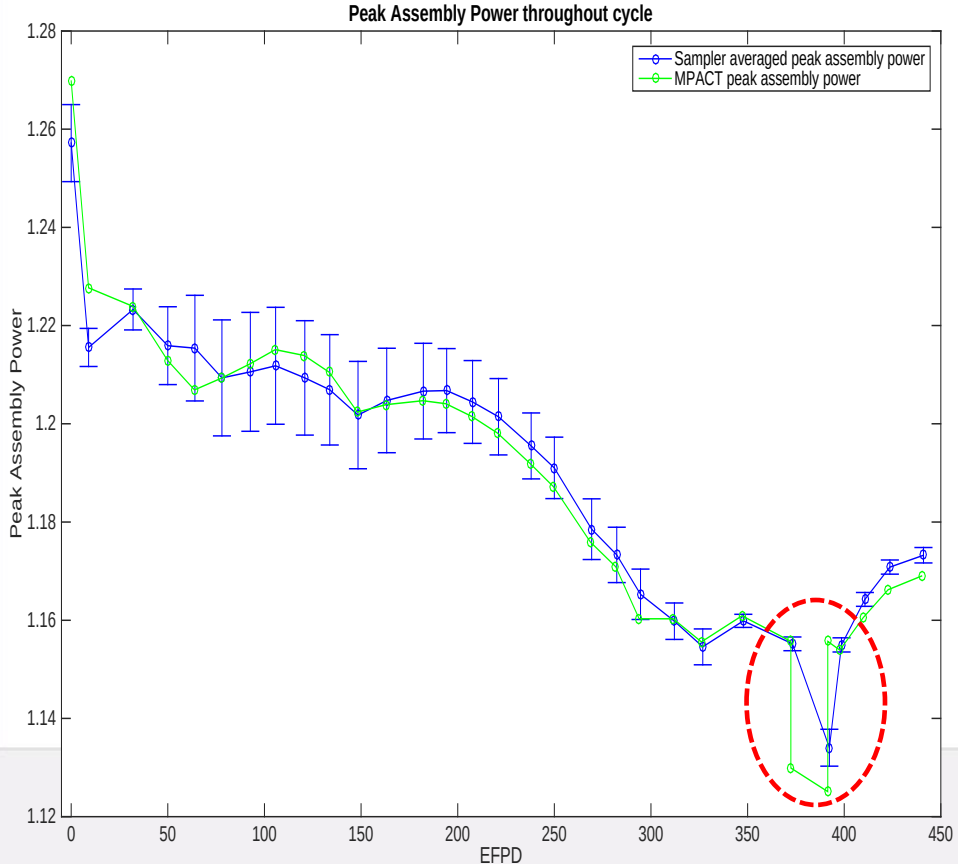


Sampler/Polaris/PARCS: Cycle 1 Critical Boron Uncertainty



EFPD	Measured Boron (ppm)	PARCS/Polaris Boron	Error (ppm)	Std. (ppm)
32.0	858	828.9	-29.1	53.5
50.0	843	829.9	-13.1	53.3
78.0	823	800.4	-22.6	53.1
105.8	790	761	-29	52.8
133.8	742	714	-28	52.7
194.3	592	588.8	-3.2	52.3
250.0	458	451.2	-6.8	52.0
282.3	370	369.1	-0.9	51.8
312.1	271	275	4	51.6
326.8	235	234.2	-0.8	51.6
373.2	95	88.1	-6.9	51.3
392.3	38	46.5	8.5	49.4
410.7	9	0.1	-8.9	39.8

Sampler/POLARIS/PARCS vs MPACT Cycle 1 Peak Assembly Power



- Measurement not available; comparison to MPACT (transport)
- Axially integrated radial power. MPACT data lies within error margins of PARCS/Sampler/Polaris results.
- Partial shutdown around 375 EFPD modelled slightly differently in PARCS.

Conclusions & Discussion

- Confidence in POLARIS/TRITON-GenPMAXS-PARCS Sequence
- Work has begun to develop POLARIS XS for Hatch (BWR)
  - Well-validated PARCS-PATHS simulation using other XS sources
- Sampler Based UQ sequence well tested
- Plan to expand detector and pin power calculation support soon
- Confidence in overall approach and results

Acknowledgements

- Matt Jessee (ORNL)
  - Setup and executed the UQ sequences in SCALE
- Kevin Xu (UM)
  - Evaluated the UQ XS with PARCS
  - Developed presentation material