ORNL EGAMCT Benchmark Phase I Results

October 25, 2013

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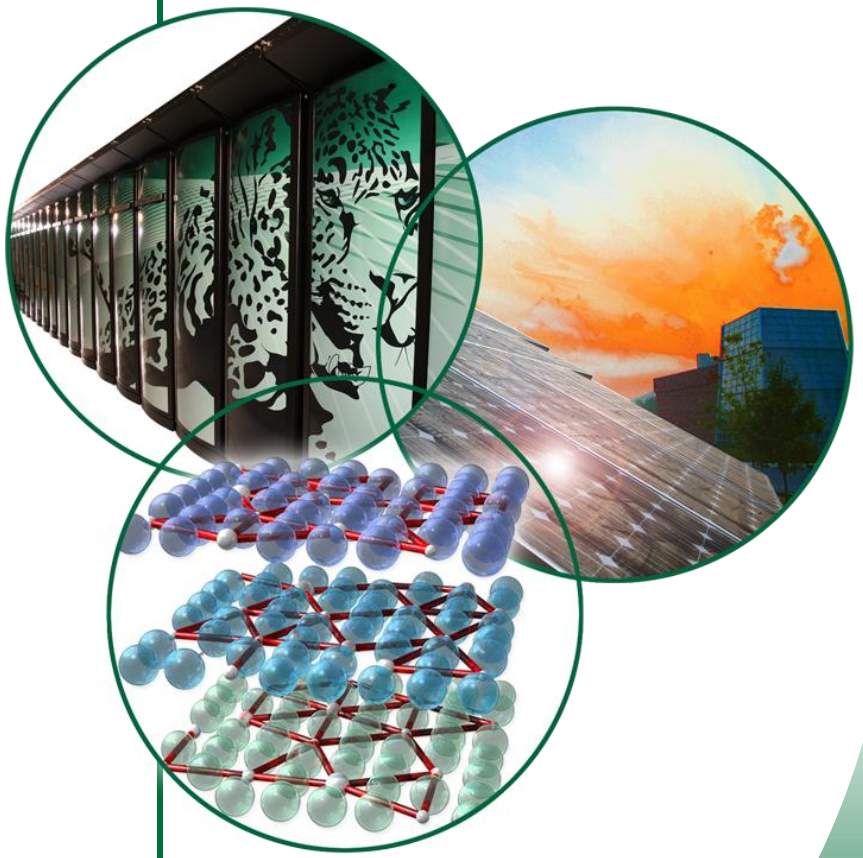


Working Party on Nuclear Criticality Safety: Expert Group on Advanced Monte Carlo Techniques

Purpose:

1. To investigate how undersampling causes eigenvalue biases, reaction rate tally biases, and poor tally variance estimates.
2. To estimate the magnitude, prevalence, and impact of these biases.
3. Produce a set of recommendations and best practices for obtaining reliable Monte Carlo reaction rate estimates in models of complex systems (i.e. Monte Carlo depletion calculations).

Approach:

- Generate models of systems relevant to burnup credit applications with varying degrees of geometric and fuel isotopic complexity.
- Simulate these models using a constant number of active histories in different NPG/GEN combinations.
- Examine how eigenvalue and flux tallies change with NPG/GEN to determine the behavior of biases in these parameters.
- Repeat these simulations multiple times to obtain “true” variance estimates.

Cases Examined

Two cases are examined in the study, each with three configurations of differing complexity:

1. PWR Core

Configuration	ID	Geometry	Isotopics	Temperature	Reaction Tally Locations
2D Quarter Core	R1	17x17 quarter core radial slice	Uniform 20 GWD/MTU with equilibrium Xenon	Reactor – Uniform Mid-Plane	Center and edge bundles
3D Core Assembly	R2	17x17 bundle in infinite lattice	18 axial zones; varying 20 GWD/MTU with equilibrium Xenon	Reactor – 18 Axial zones	Top, mid-plane, and bottom
3D Quarter Core	R3	17x17 quarter core	18 axial zones; 20 GWD/MTU with equilibrium Xenon; Uniform radially	Reactor – Uniform radially, 18 axial zones	Center and edge bundles Top, mid-plane, and bottom

2. Used Fuel Shipping Cask

Configuration	ID	Geometry	Isotopics	Temperature	Reaction Tally Locations
2D Storage Cask	S1	17x17 in cask geometry radial slice	Uniform 40 GWD/MTU with 5 year cooling time	Uniform storage temperature	Center and edge bundles
3D Cask Assembly	S2	17x17 bundle in infinite lattice	18 axial zones; 40 GWD/MTU with 5 year cooling time	Uniform storage temperature	Top, mid-plane, and bottom
3D Cask	S3	17x17 in full cask	18 axial zones; 40 GWD/MTU with 5 year cooling time; Uniform radially	Uniform storage temperature	Center and edge bundles Top, mid-plane, and bottom

Scope of the Study

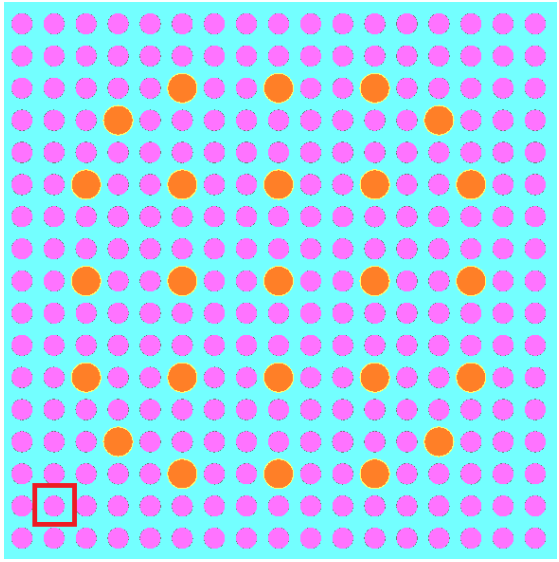
- Each of the six benchmark cases were simulated using a constant number of active histories and different combinations of the number of particles per generation (NPG) and the number of active generations (GEN).
- Each simulation used 100 million active histories and was repeated 30 times using different random seeds per NPG/GEN combination (for a total of 3 billion active histories per data point).
- "Normalized" Pin Flux tallies were calculated to allow for pcm comparisons between pin flux tallies. The Normalized Flux was obtained for each fuel pin by dividing the flux tallies for each NPG/GEN case by the flux for the 10,000 NPG/GEN case.
- All simulations used 500 skipped cycles to ensure fission source convergence.
- The work presented here represents the results of 0.5 trillion active particle histories.

Reaction Rate Tally Locations – 2D Core (R1)

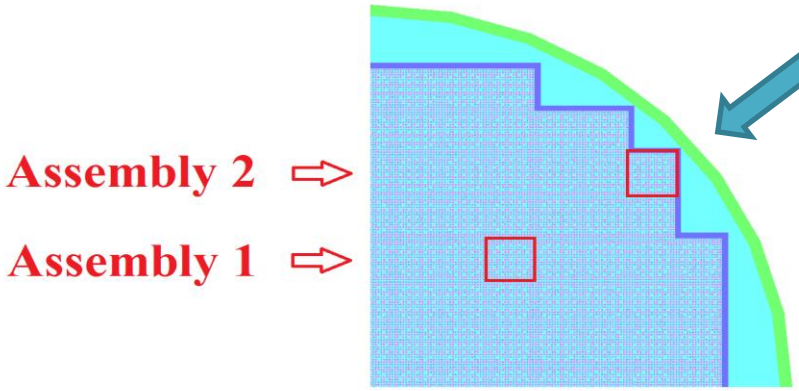
Pin 0 = All fuel pins
(Very good statistics, σ ≈ 0.001%)

Pin 1 = Fuel pin in an assembly in the middle of the quarter-core.
(Good statistics, σ ≈ 0.05%)

Pin 2 = Fuel pin in an assembly near the edge of the quarter-core.
(Poor statistics, σ ≈ 0.10%)



Fuel Pin Location in each Assembly

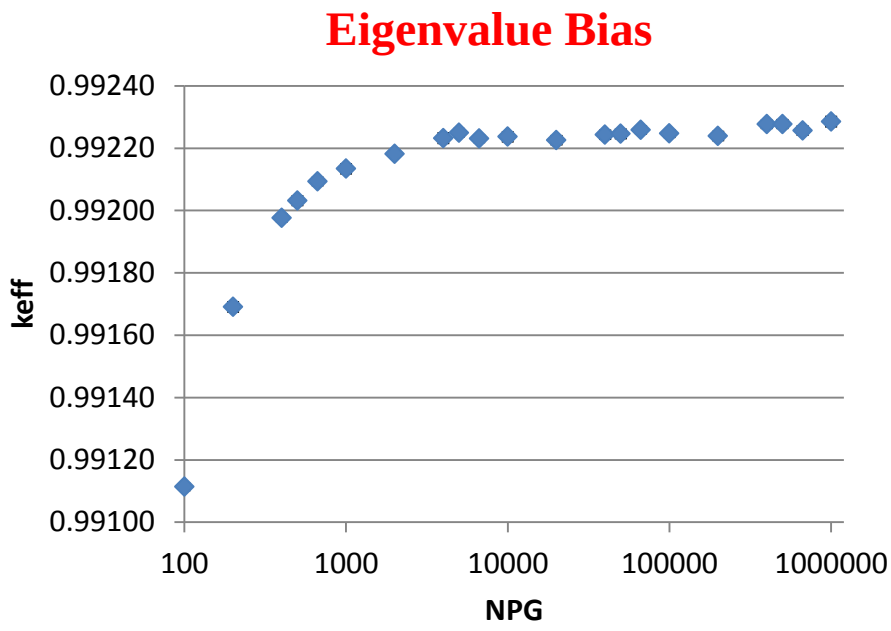


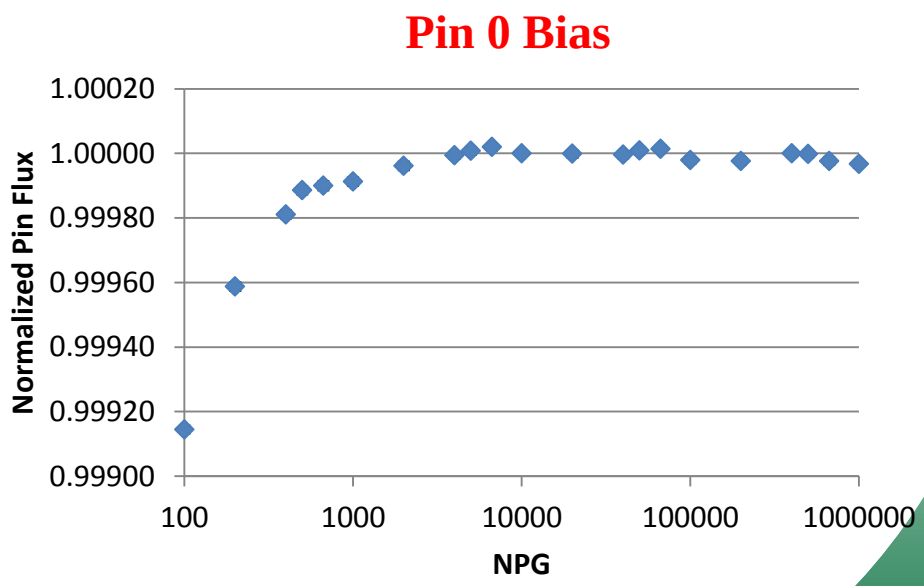
Assembly Locations

2D Core (R1) Bias Examination

- The eigenvalue bias was relatively small for the 2D Core model, having a total range of about 100 pcm.

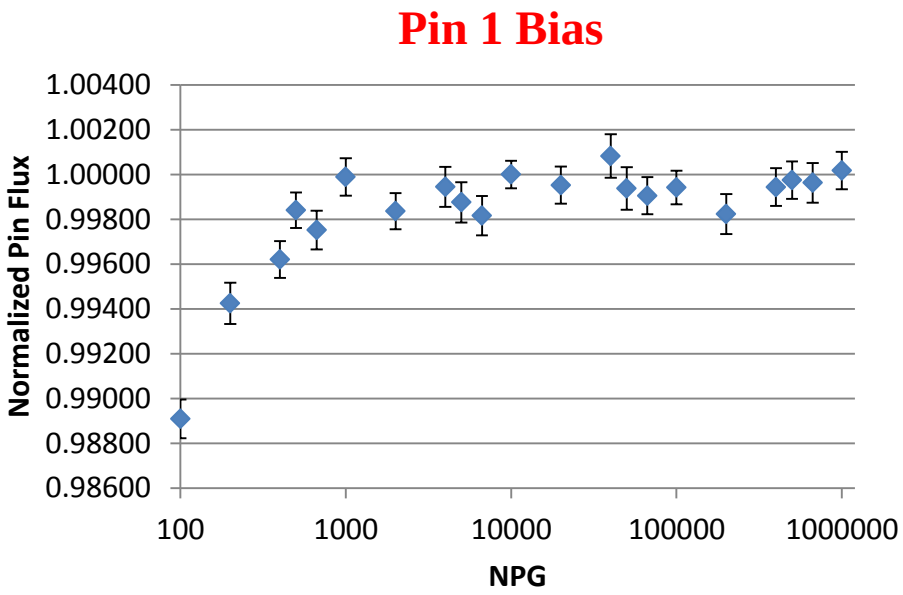
- The **Pin 0** bias range was also about 100 pcm.

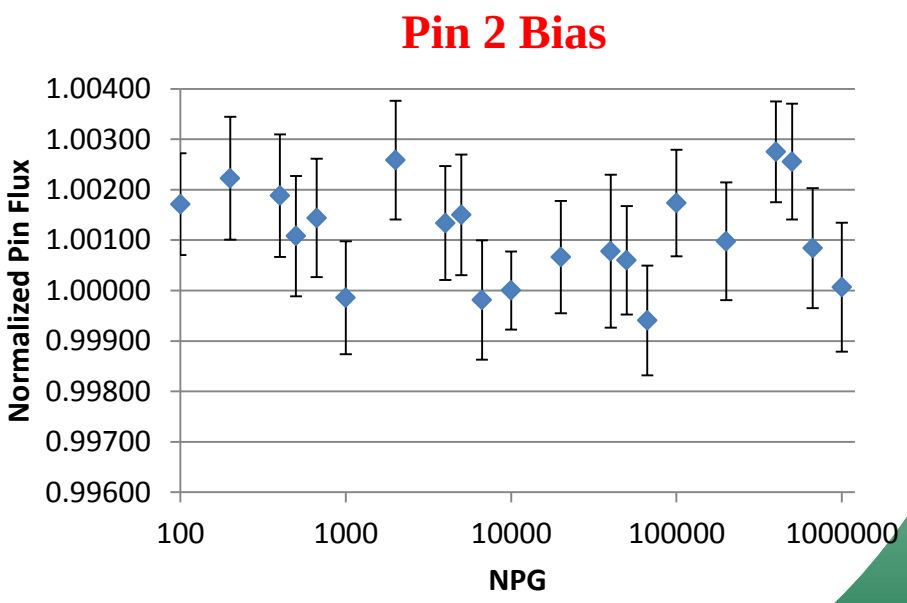




2D Core (R1) Bias Examination

- The **Pin 1** bias was more substantial, having a range of about 1200 pcm.
- The **Pin 2** bias was also substantial (several hundred pcm), but the larger individual tally uncertainty made it difficult to ascertain bias behavior.
- These results suggest a minimum of NPG=4000 to minimize the occurrence of biases.
- Future simulations will likely require more active histories (or more repeated calculations) to reduce the tally uncertainty.



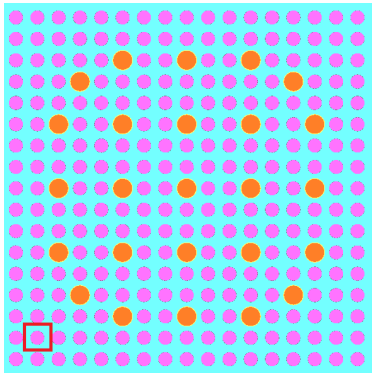


Reaction Rate Tally Locations – 3D Core Assembly (R2)

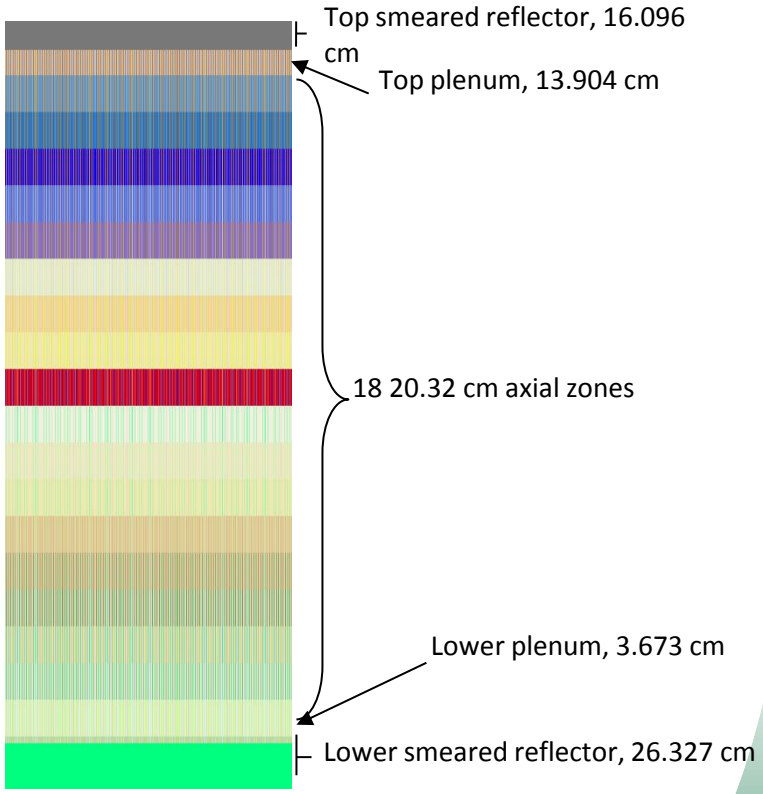
Pin 1 = Fuel pin in an axial slice 3/4'ths up the assembly.
(Good statistics, σ ≈ 0.25%)

Pin 2 = Fuel pin in an axial slice in the middle of the assembly.
(Good statistics, σ ≈ 0.15%)

Pin 3 = Fuel pin in the bottom axial slice.
(Decent statistics, σ ≈ 0.45%)



Fuel Pin Location in each Assembly

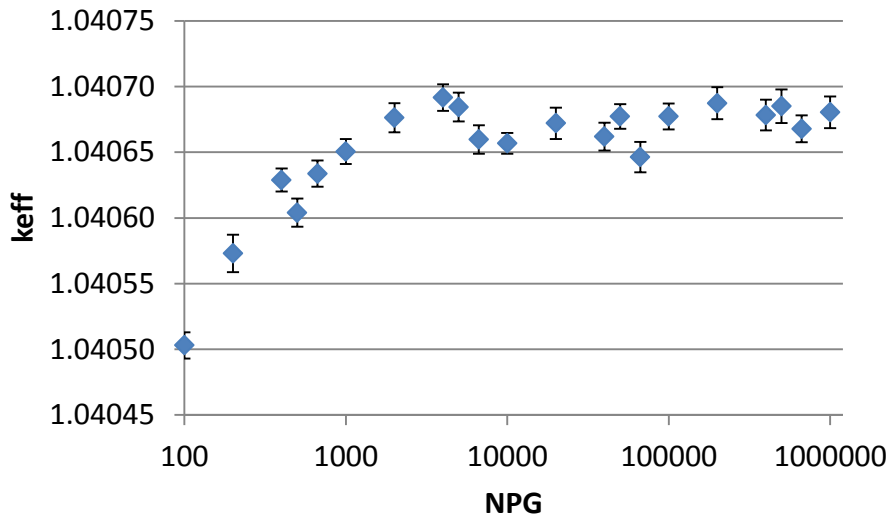


Assembly Axial Slices

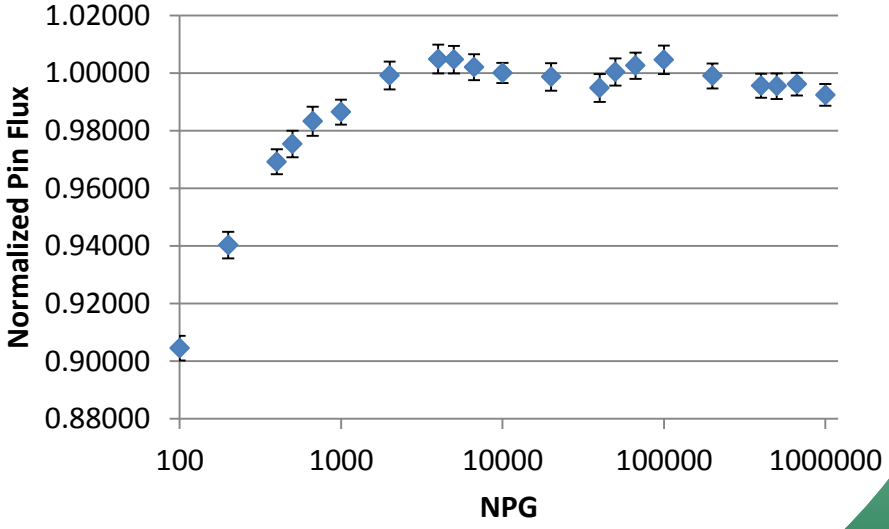
3D Core Assembly (R2) Bias Examination

- The eigenvalue bias was even smaller than the **2D Core** bias, having a total range of about 20 pcm.
- The **Pin 1** flux bias range was much larger than for the **2D Core** flux biases, having a range of nearly 12% (12,000 pcm).

Eigenvalue Bias

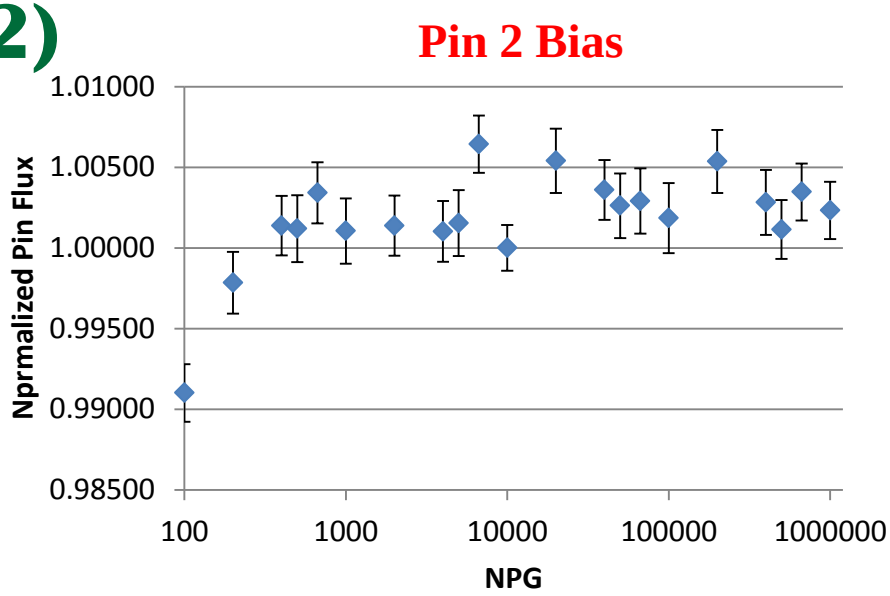


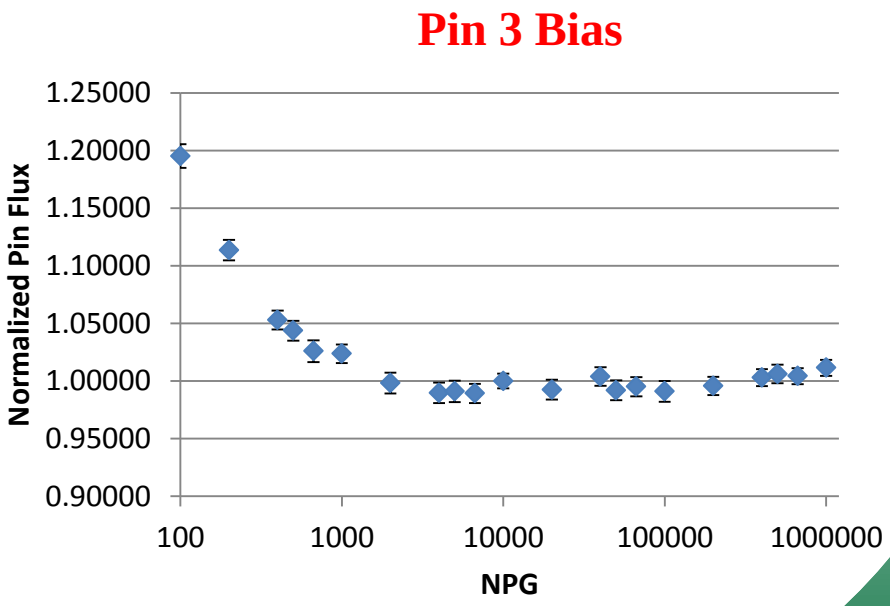
Pin 1 Bias



3D Core Assembly (R2) Bias Examination

- The **Pin 2** bias was not as large as the **Pin 1** and **Pin 3** biases, but was still substantial (1,500 pcm).
- The **Pin 3** had the bias was very large, having a range of nearly 20% (20,000 pcm!) This bias was still several percent in magnitude for NPG=1000.
- Again, the biases seem to disappear once NPG=4000 is used.



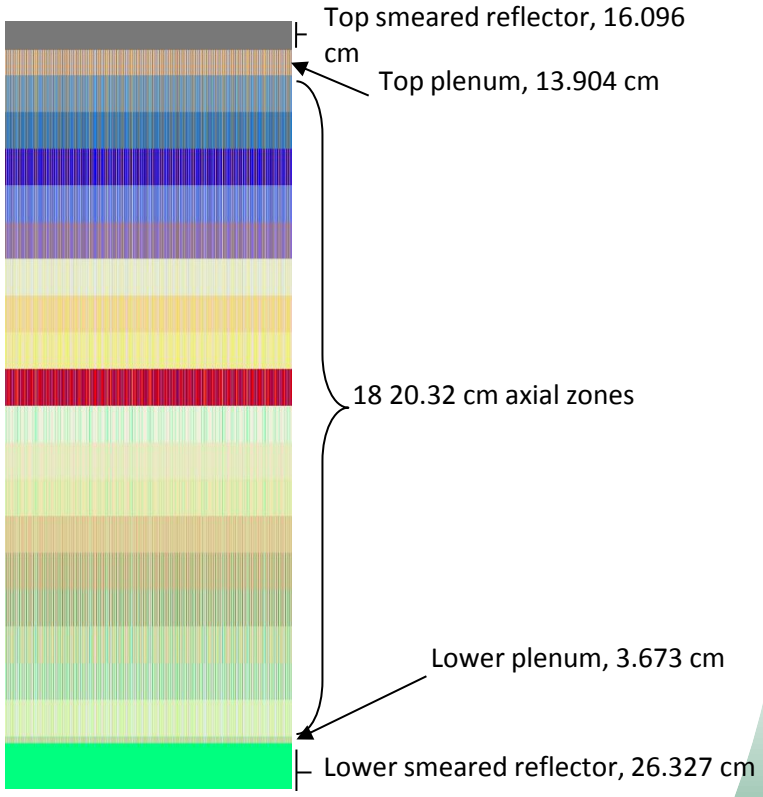


Reaction Rate Tally Locations – 3D Core (R3)

Pin 1 = Fuel pin in an assembly near the top-edge of the quarter-core.
(Good statistics, σ ≈ 1.0%)

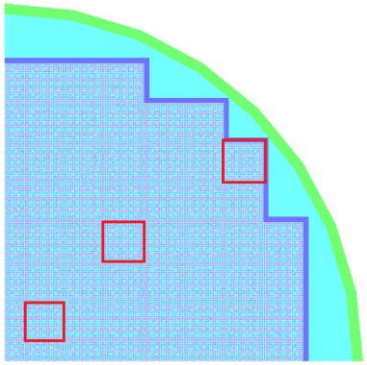
Pin 2 = Fuel pin in an assembly in the middle of the quarter-core.
(Very good statistics, σ ≈ 0.3%)

Pin 3 = Fuel pin in an assembly in the bottom-center of the quarter-core.
(Good statistics, σ ≈ 1.0%)



Assembly Axial Slices

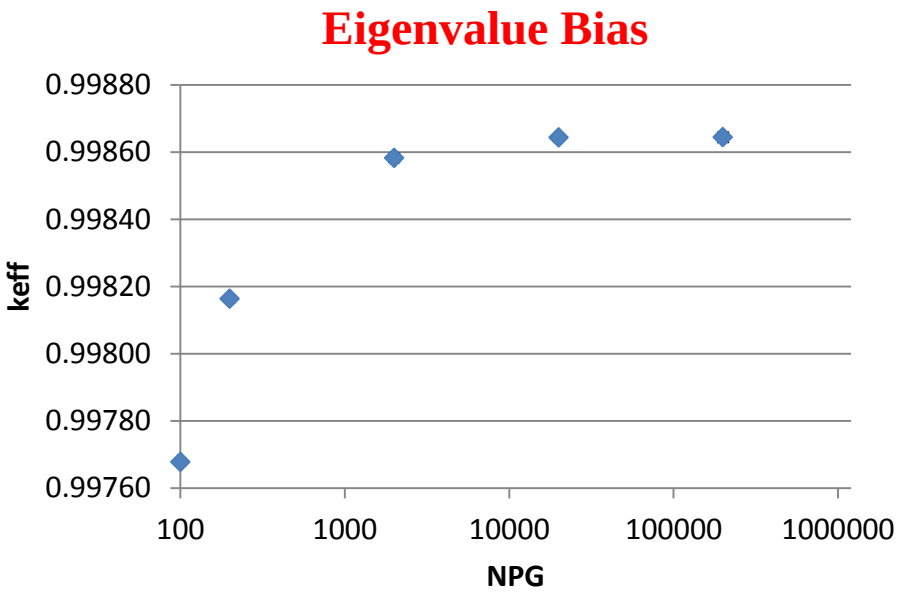
Assembly 1 ⇨
Assembly 2 ⇨
Assembly 3 ⇨

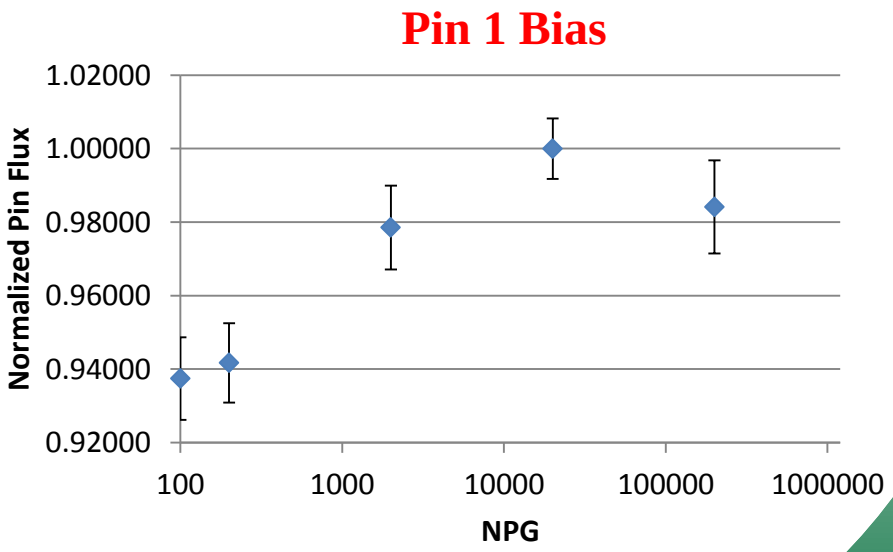


Assembly Locations

3D Core (R3) Bias Examination

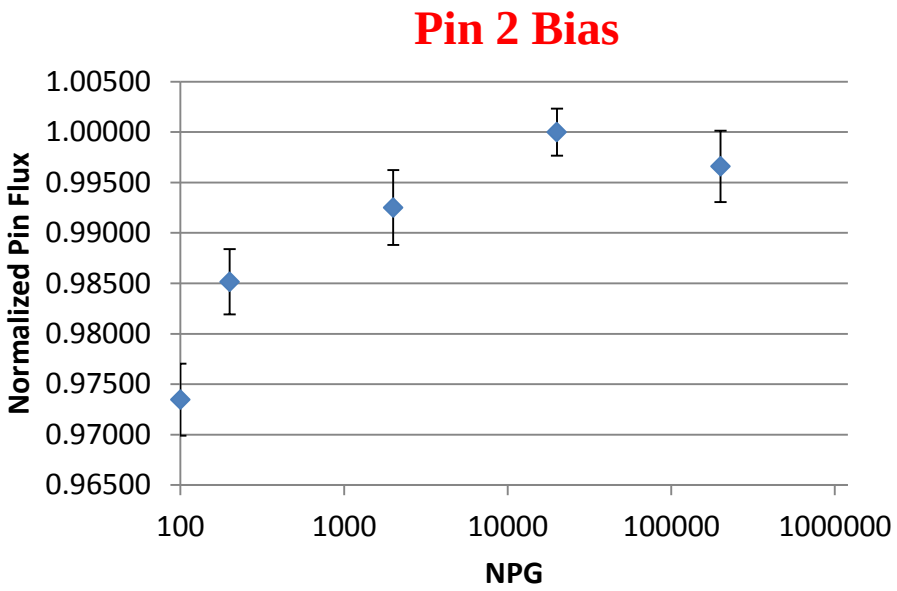
- Due to time constraints, the **3D Core** and **3D Cask** cases could not use as many NPG/GEN data points as the other cases.
- The eigenvalue bias was about the same size as the **2D Core** bias, having a total range of about 100 pcm.
- The **Pin 1** flux bias range seems to be about 6% (6000 pcm), but statistical uncertainty makes it difficult to determine the true magnitude of this bias.

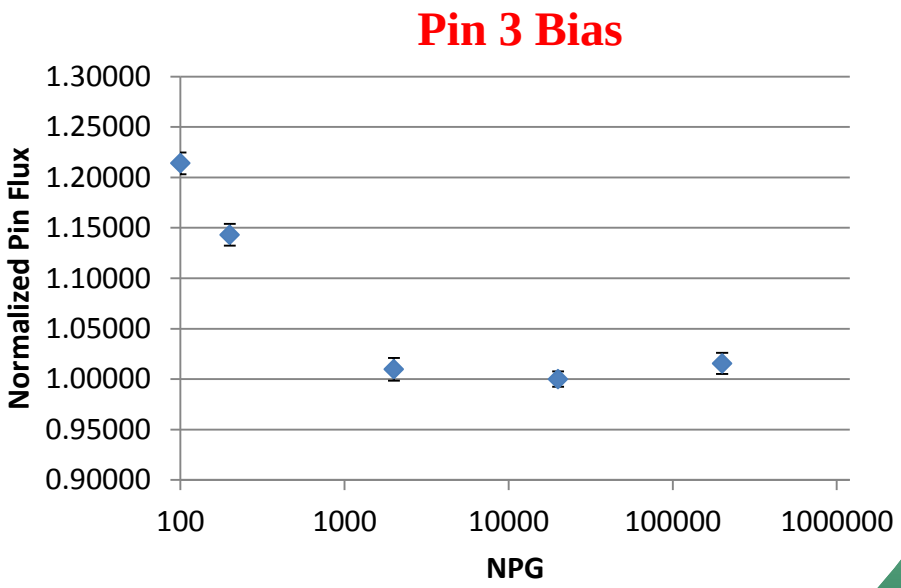




3D Core (R3) Bias Examination

- The **Pin 2** bias was not as large as the **Pin 1** and **Pin 3** biases, but was still substantial (2500 pcm).
- The **Pin 3** had the bias was very large and had a range of nearly 25% (20,000 pcm). This bias was even larger than the bias observed for fuel pins near the bottom of the **3D Core Assembly** case.
- Again, the biases seem to disappear once several thousand particles are simulated per generation.



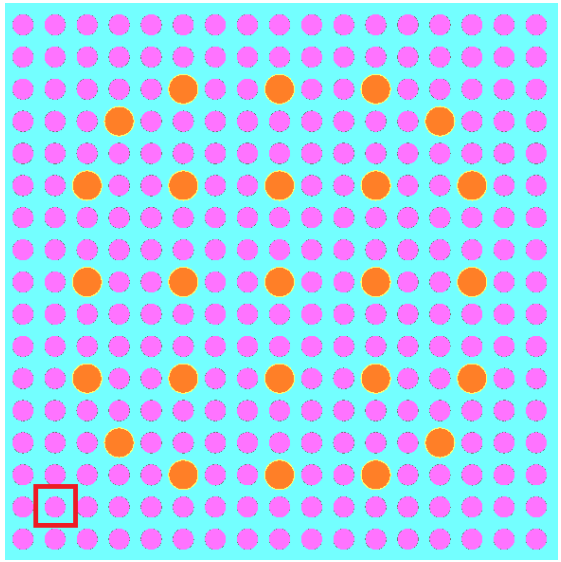


Reaction Rate Tally Locations – 2D Cask (S1)

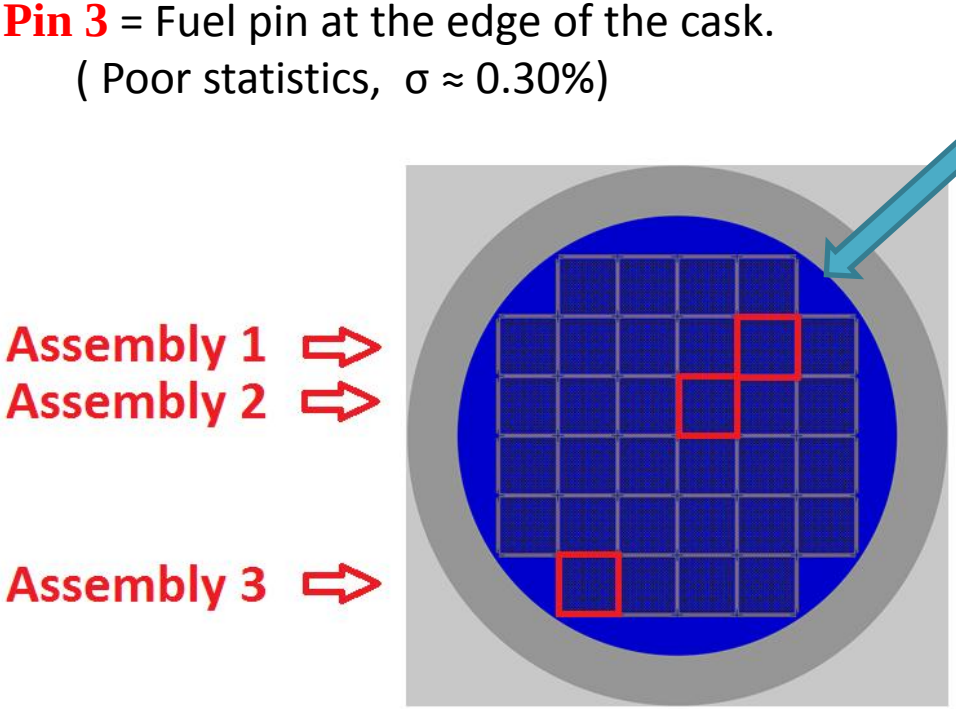
Pin 1 = Fuel pin in an assembly near the edge of the cask.
(Good statistics, σ ≈ 0.15%)

Pin 2 = Fuel pin in an assembly in the middle of the cask.
(Good statistics, σ ≈ 0.10%)

Pin 3 = Fuel pin at the edge of the cask.
(Poor statistics, σ ≈ 0.30%)



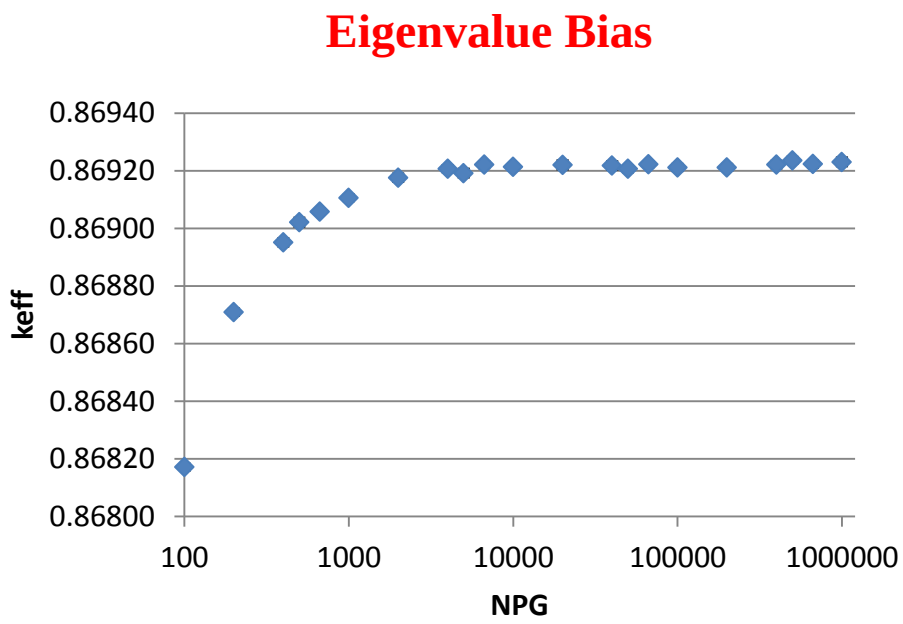
Fuel Pin Location in each Assembly

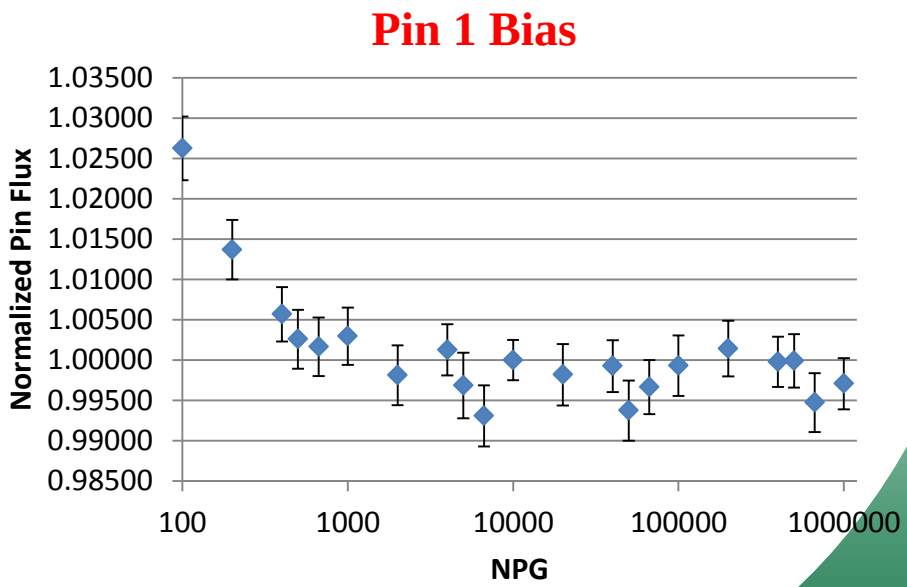


Assembly Tally Locations

2D Cask (S1) Bias Examination

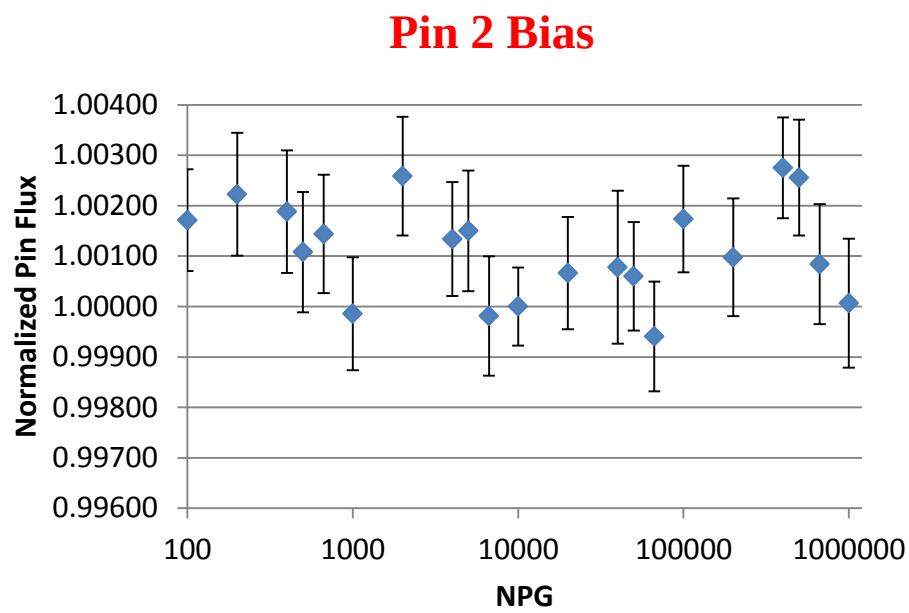
- The eigenvalue bias for the **2D Cask** model was about 100 pcm.
- The **Pin 1** bias was about 2.5% (2500 pcm), which was significantly larger than the biases observed for the **2D Core** model.
- The **Pin 0** bias (not shown) again had a range of about 120 pcm, which was about equal to the magnitude of the eigenvalue bias.

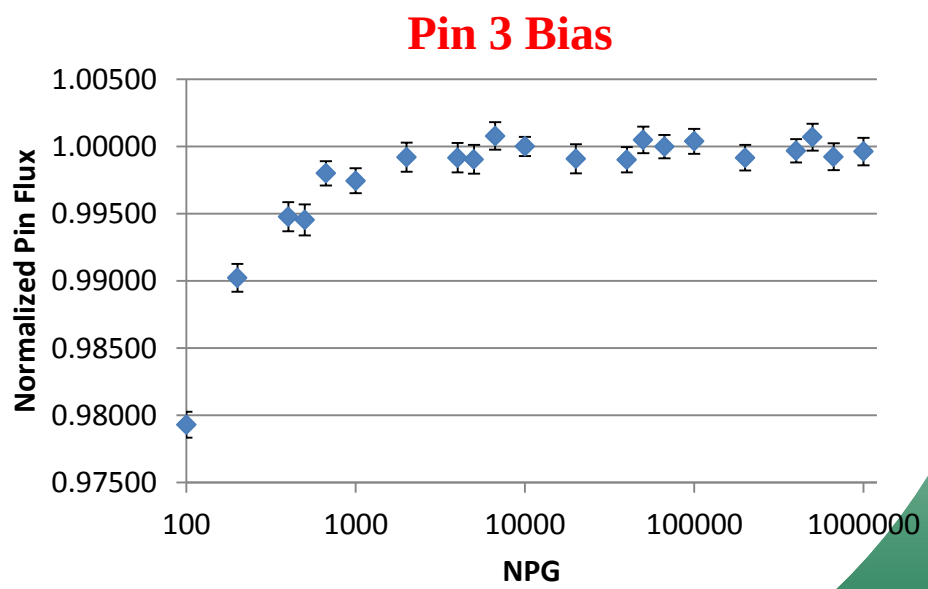




2D Cask (S1) Bias Examination

- **Pin 3** showed a bias range of about 2% (2000 pcm), which was similar to the bias range of **Pin 1**.
- The **Pin 2** bias was not significant given the statistical uncertainty of its flux tallies.
- These results again suggest a minimum of NPG=4000 to minimize the occurrence of biases.



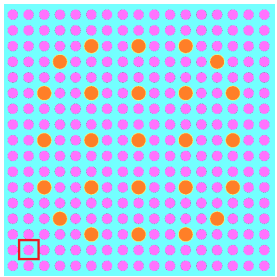


Reaction Rate Tally Locations – 3D Cask Assembly (S2)

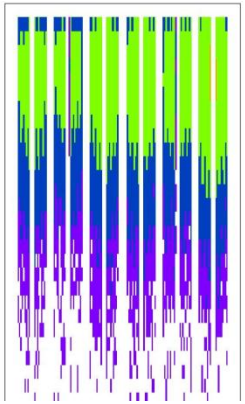
Pin 1 = Fuel pin in an axial slice 17/18ths up the assembly.
(Good statistics, σ ≈ 0.04%)

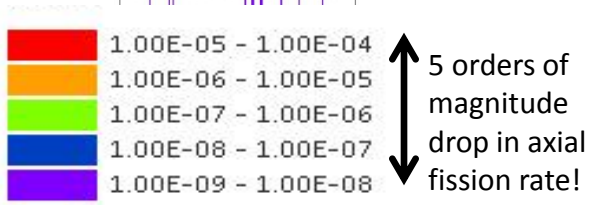
Pin 2 = Fuel pin in an axial slice in the middle of the assembly.
(Good statistics, σ ≈ 0.60%)

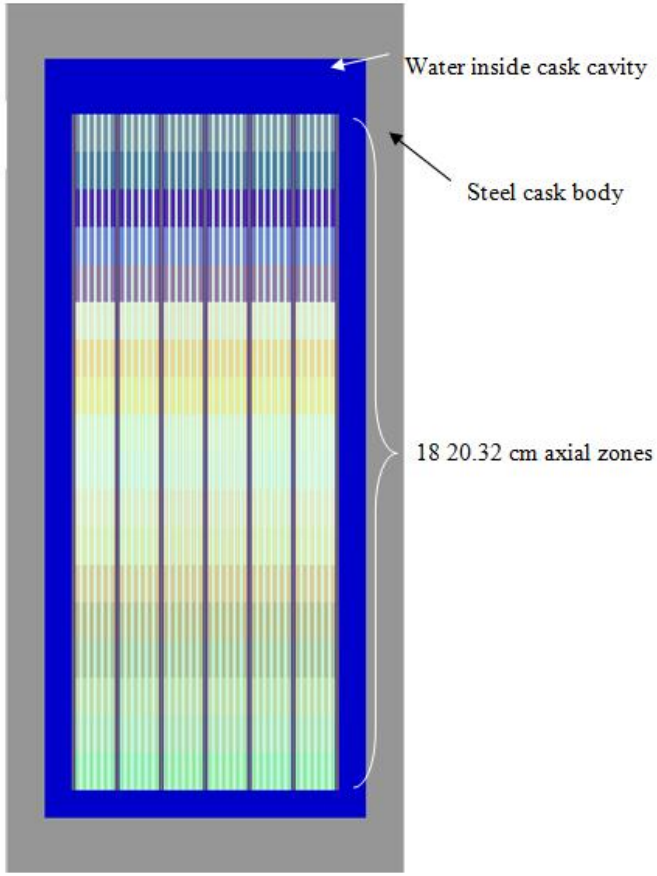
Pin 3 = Fuel pin in the second-to-bottom axial slice.
(Terrible statistics, σ ≈ 30%)



Fuel Pin Location in each Assembly



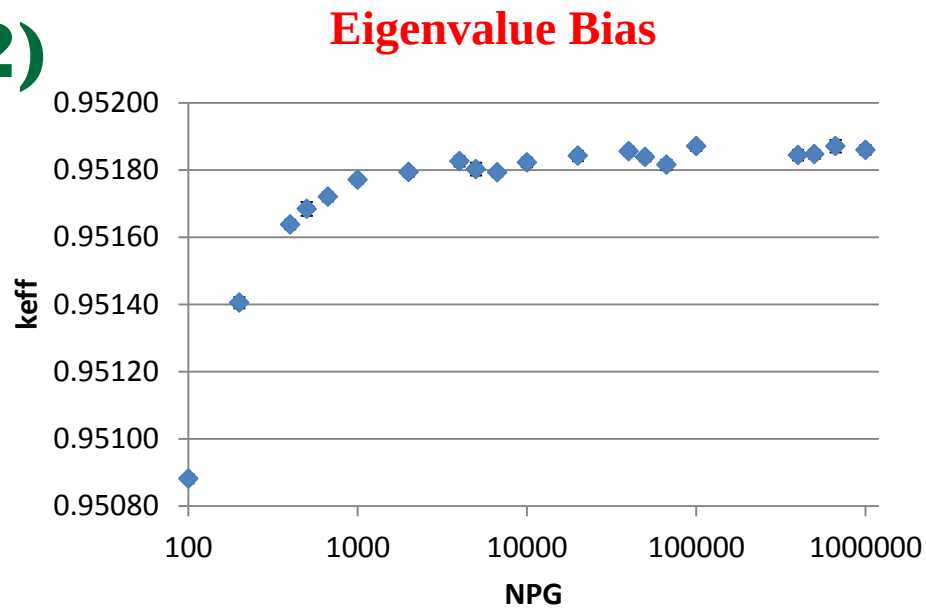


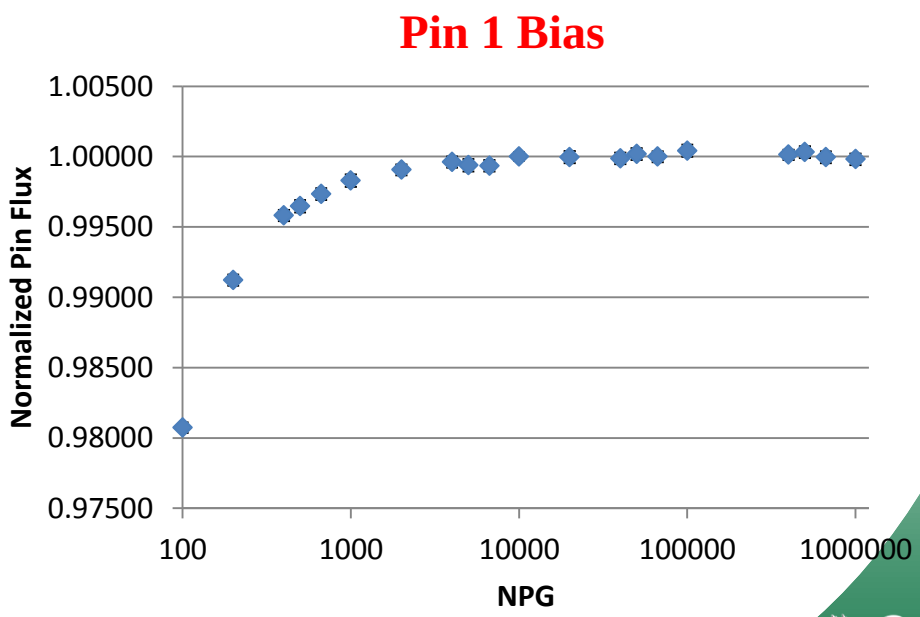


Assembly Axial Slices

3D Cask Assembly (S2) Bias Examination

- The eigenvalue bias was again about 100 pcm, which was significantly larger than the bias observed for the **3D Core Assembly** case.
- All **3D Cask Assembly** fuel pin flux tallies produced significant biases.
- **Pin 1** showed a bias range of about 2% (2000 pcm), which was surprising given that this pin has the highest fission rate.

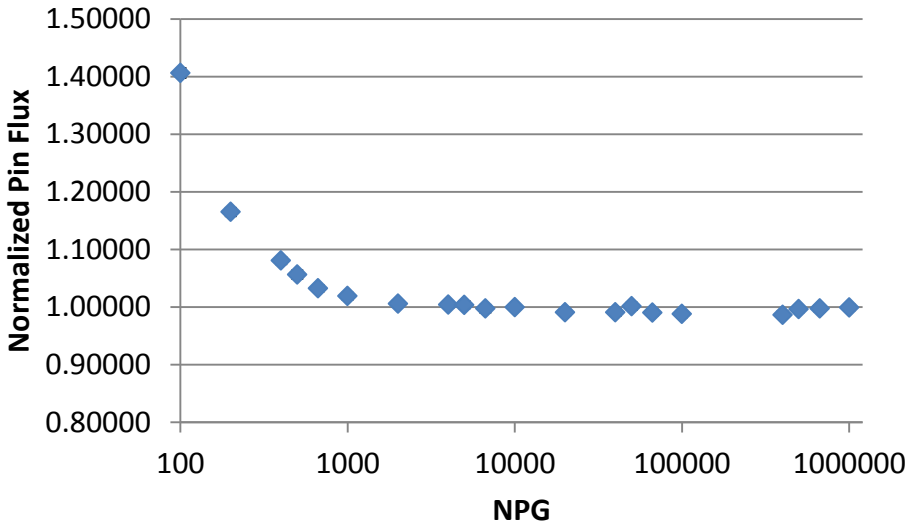




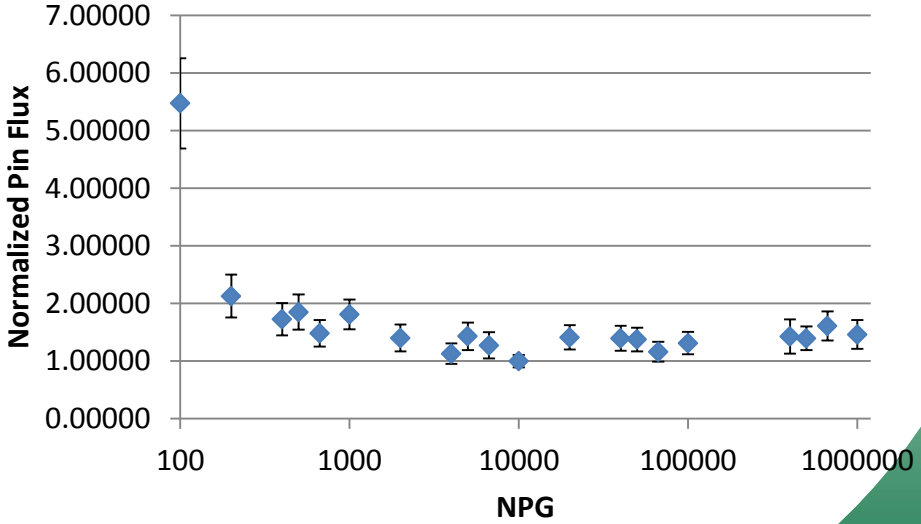
3D Cask Assembly (S2) Bias Examination

- The **Pin 2** and **Pin 3** biases were much more significant than the **Pin 1** biases.
- The **Pin 2** biases had a range of 40% (40,000 pcm), and a downward trend in the normalized pin fluxes is visible between 1,000 and 100,000 NPG.
- The **Pin 3** bias was one of the largest of any fuel pin in this study, and low NPG cases disagreed by several hundred percent.

Pin 2 Bias



Pin 3 Bias

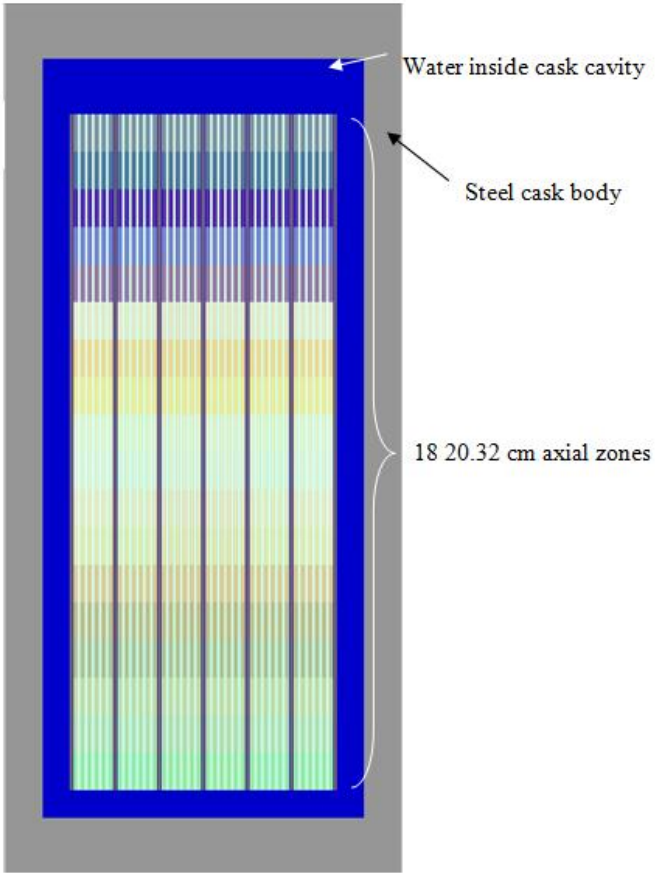


Reaction Rate Tally Locations – 3D Cask (S3)

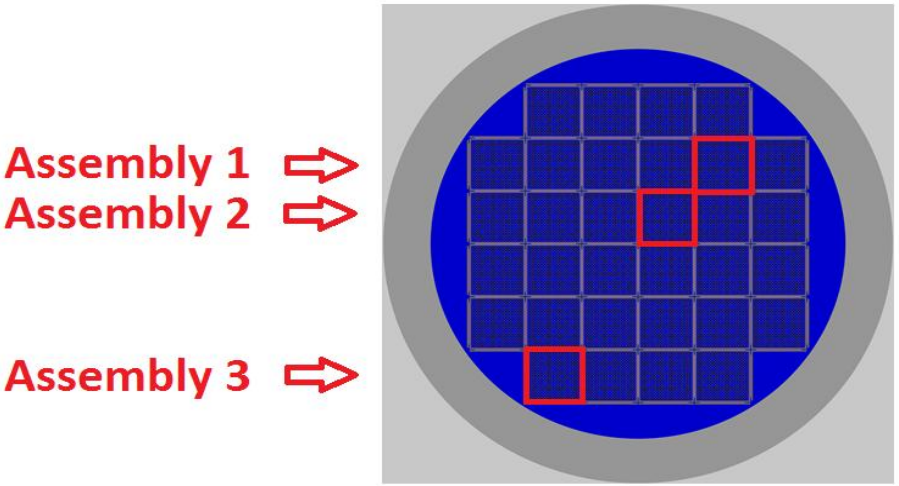
Pin 1 = Fuel pin in an assembly near the top-edge of the cask.
(Good statistics, σ ≈ 0.25%)

Pin 2 = Fuel pin in an assembly in the middle of the cask.
(Decent statistics, σ ≈ 1.5%)

Pin 3 = Fuel pin at the bottom-edge of the cask.
(Terrible statistics, σ ≈ 50%)



Cask Axial Slices

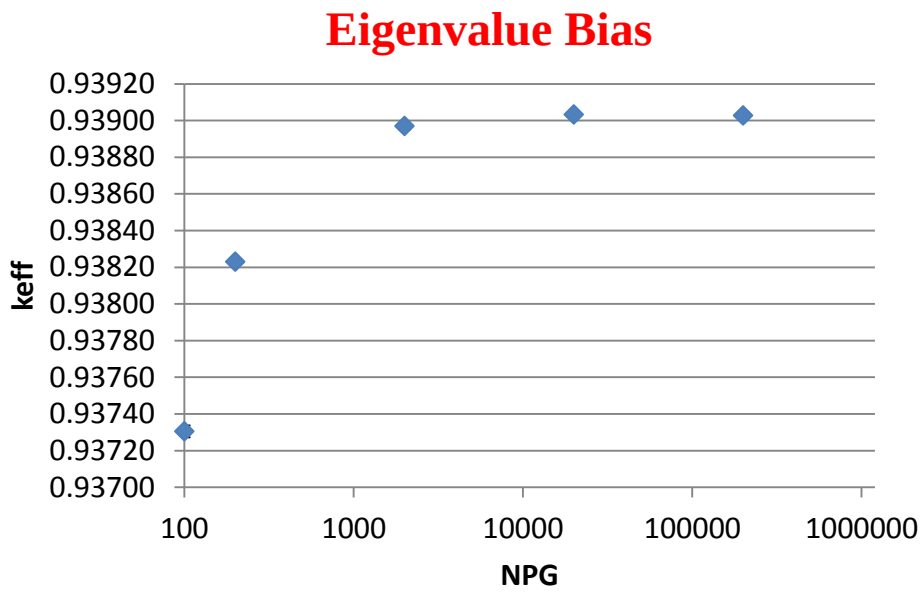


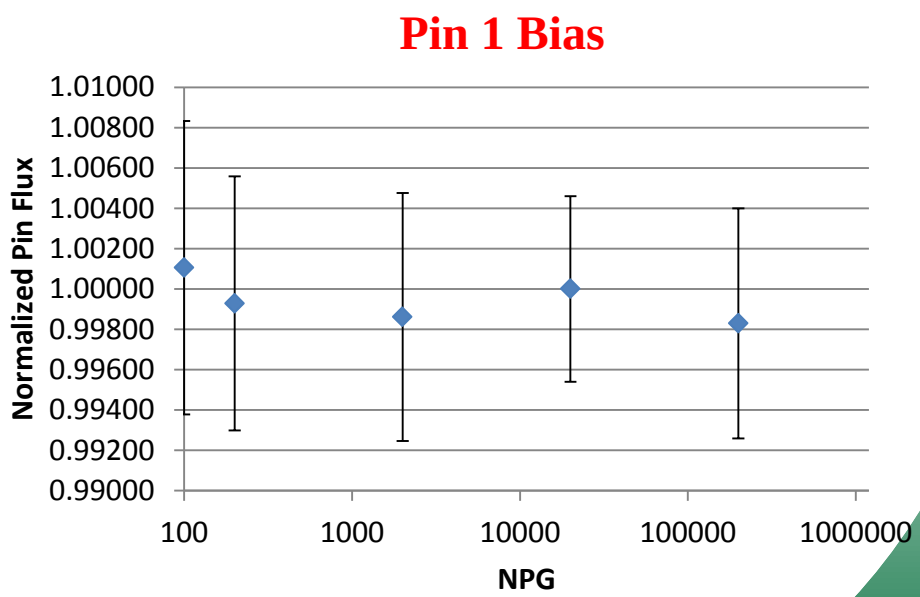
Assembly Tally Locations

3D Cask (S3) Bias Examination

- The eigenvalue bias was about 200 pcm, which was about twice as large as the biases observed for the **2D Cask** and **3D Cask Assembly** cases.

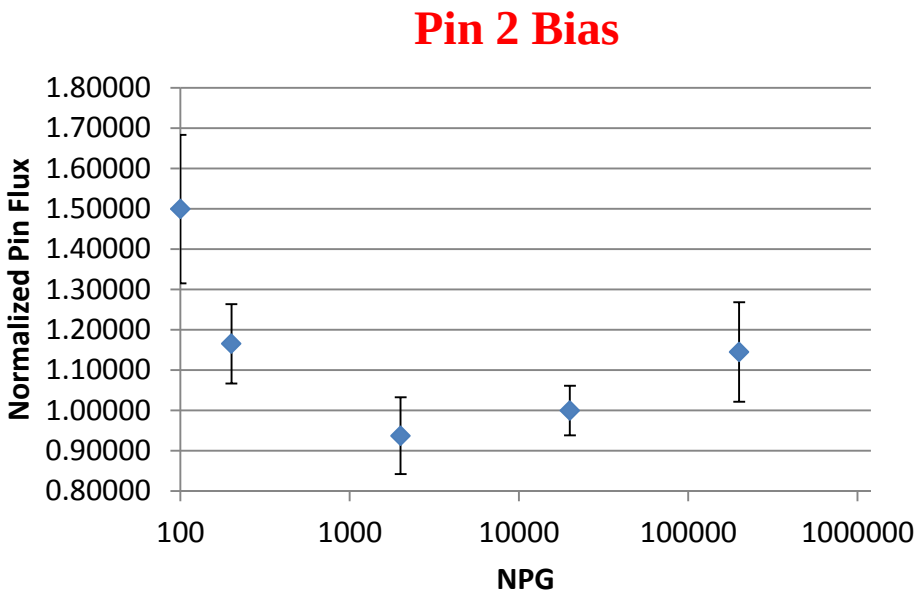
- All **3D Cask** fuel pin flux tallies seem to have produced significant biases, but the large statistical uncertainty of these tallies makes it difficult to truly identify these biases.

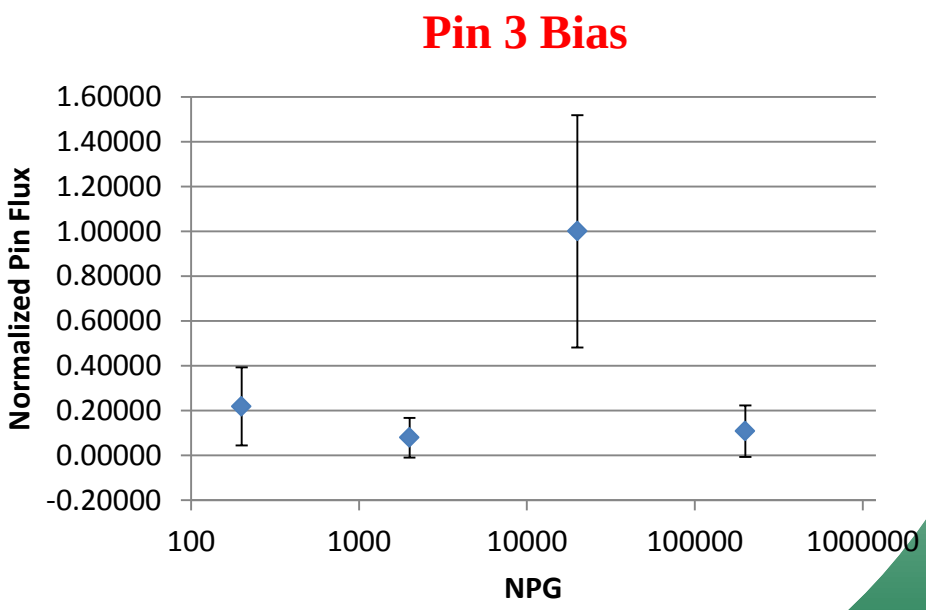




3D Cask (S3) Bias Examination

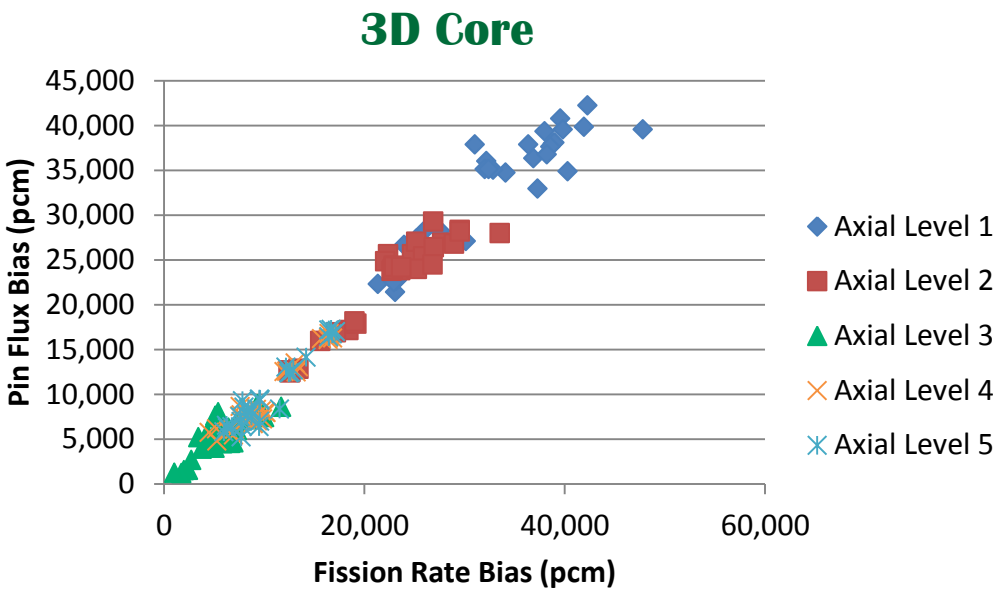
- The **Pin 2** results suggested a bias of tens of percent, but the large statistical uncertainty of these tallies makes these results inconclusive.
- The **Pin 3** results show obvious biases, but the large amount of statistical uncertainty in these tallies makes it impossible to quantify the magnitude of these biases.
- Any study seeking to obtain the **Pin 3** flux tallies at a 1% statistical uncertainty would need to simulate an expected 20 **trillion** particle histories.



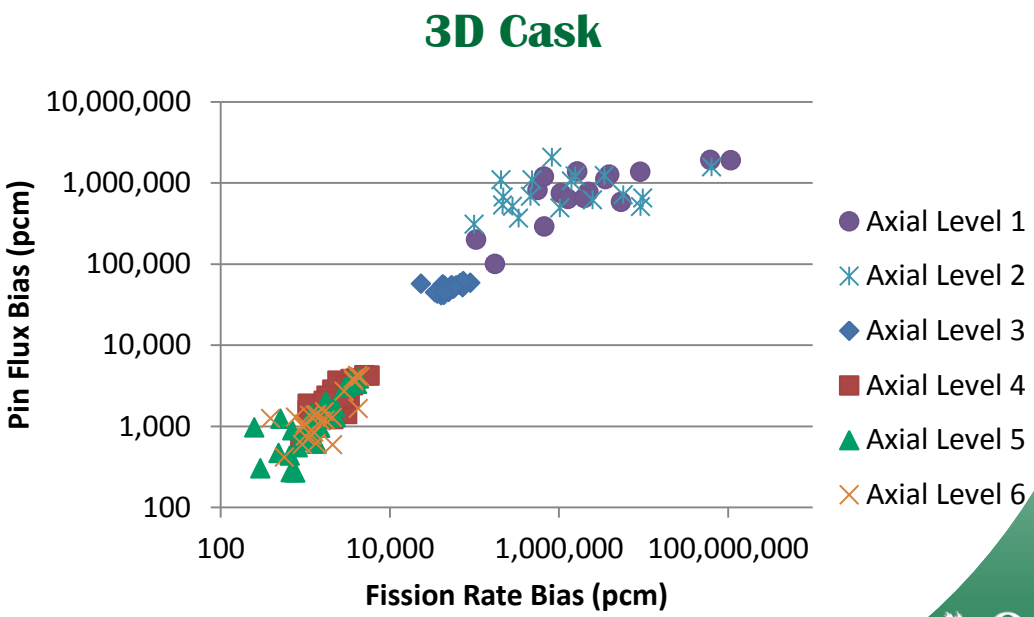


Fission Rates

- This study also briefly examined biases in fuel pin fission rates.



- As expected, fission rate biases are nearly proportional to fuel pin flux biases.



Conclusions and Continuing Work

- 4,000 NPG is a generally observed to be an adequate number of particles per generation to minimize the occurrence of biases in system eigenvalues and pin flux tallies.
- It is unclear what biases would be observed for more resolved tallies, such as:
  - Reaction-dependent tallies
  - Energy-dependent tallies
  - Reaction-/energy-/importance-dependent tallies (i.e. sensitivity coefficient tallies)
- Large biases certainly exist when NPG is too small, and this benchmark study needs a useful way to examine the causes of these biases and should seek to develop methods/metrics for predicting when these biases will occur.
- This study tries to do too much. Having bias information for 100+ fuel pins is not useful, it's too much information to analyze. We should focus on quantifying and predicting biases for assembly fluxes or restrict our study to examine a smaller number of fuel pins.
- In its current state, this study cannot identify biases for the **3D Cask (S3)** case. It simply requires too many active histories.