Continued Investigation of Metrics to Detect Undersampling Biases

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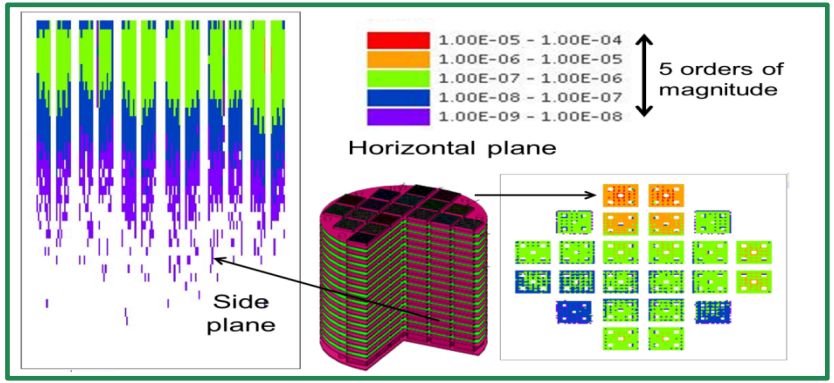
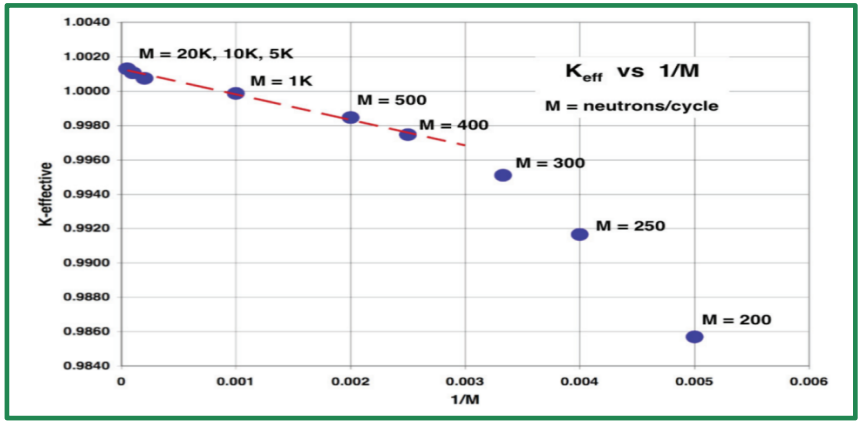
Introduction

- Brown, Mervin, and others have observed significant biases in eigenvalue estimates, flux tallies, and uncertainty estimates due to the insufficient sampling of particle histories in Monte Carlo calculations.



A spent fuel shipping cask model where the fission source varies by 5 orders of magnitude; this model is especially susceptible to the effects of undersampling (Ibrahim 2013)



Eigenvalue biases in the K-effective of the World Problem [Brown 2011]

- The Expert Group on Advanced Monte Carlo Techniques (EGAMCT) was established to understand best practices for ensuring the accuracy of flux and reaction rate calculations in several applications.

EGAMCT Benchmark Problems: Reactor Cases

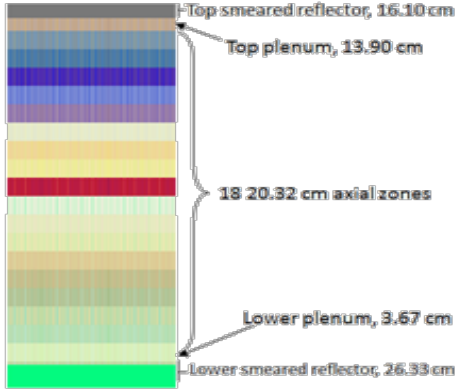
Three Benchmark Cases:

R1 = 2D Core

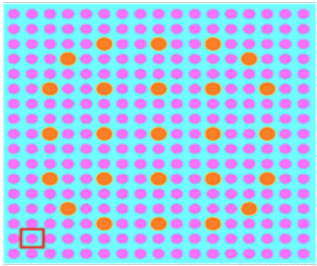
R2 = 3D Infinitely Reflected Assembly

R3 = 3D Core

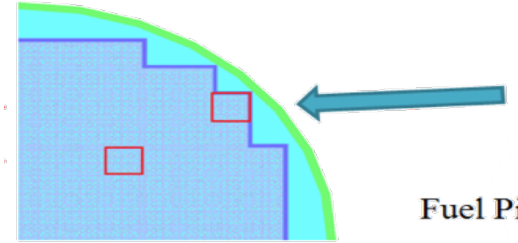
- Fuel temperature varies with axial location
- Isotopics correspond to 20 GWd/MTU fuel



Assembly Axial Slices



Fuel Pin Location in each Assembly



Assembly Locations

[Perfetti and Rearden 2014]

EGAMCT Benchmark Problems: Shipping Cask Cases

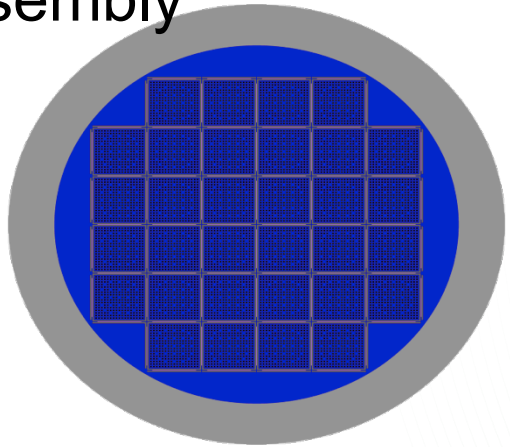
Three Benchmark Cases:

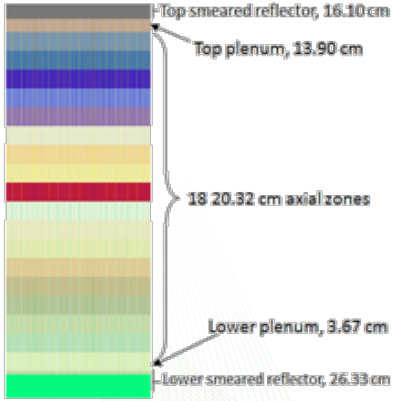
S1 = 2D Cask

S2 = 3D Infinitely Reflected Assembly

S3 = 3D Cask

- Uniform storage temperature
- Isotopics corresponding to 40 GWd/MTU fuel with a 5-year cooling time



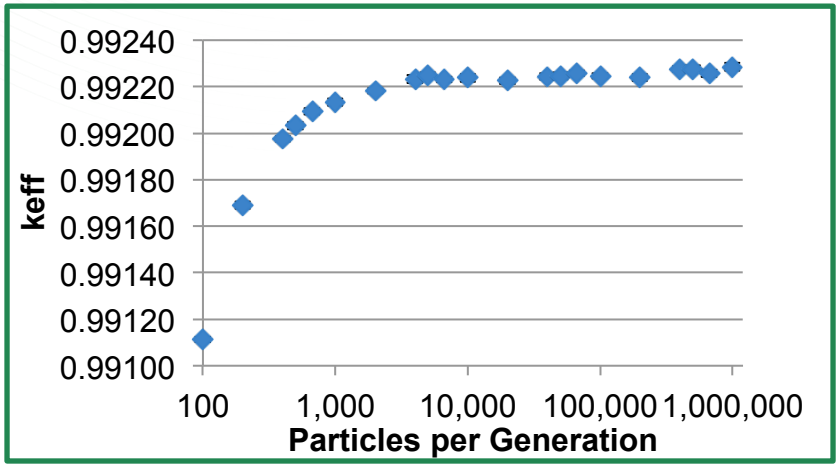


Assembly Axial Slices

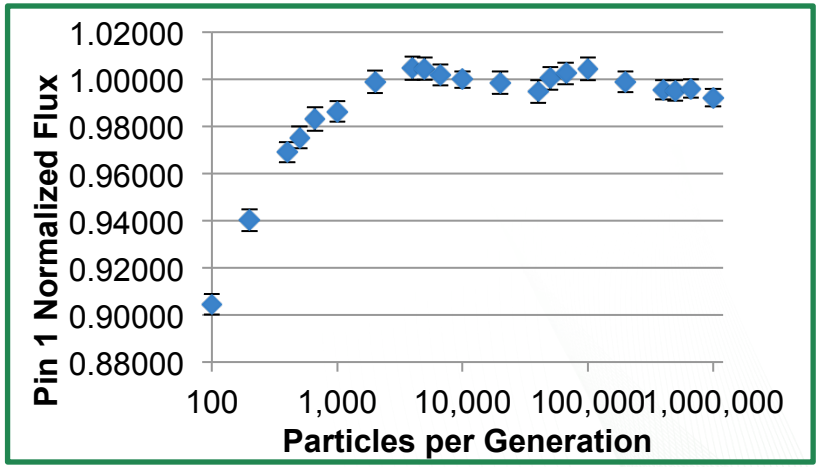
[Perfetti and Rearden 2014]

Background

- In 2013, significant undersampling biases were observed for many eigenvalue, flux, and fission rate tallies in the EGAMCT cases.
- Undersampling biases were most severe (tens of percent) for axially dependent flux tallies, even in infinitely reflected single-assembly models.



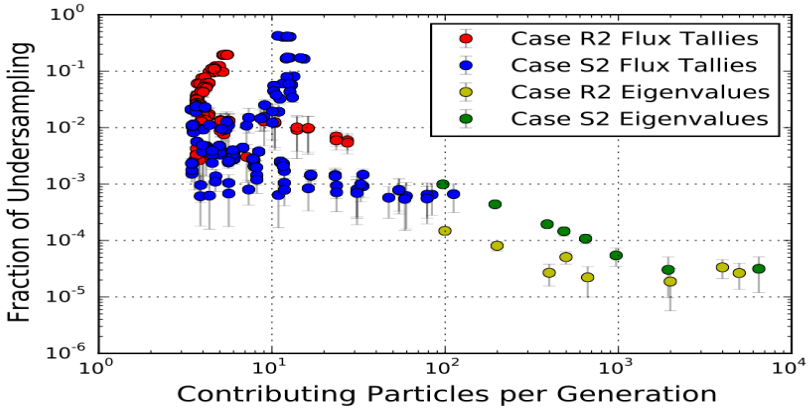
Undersampling in Case R1 eigenvalues [Perfetti and Rearden 2014]

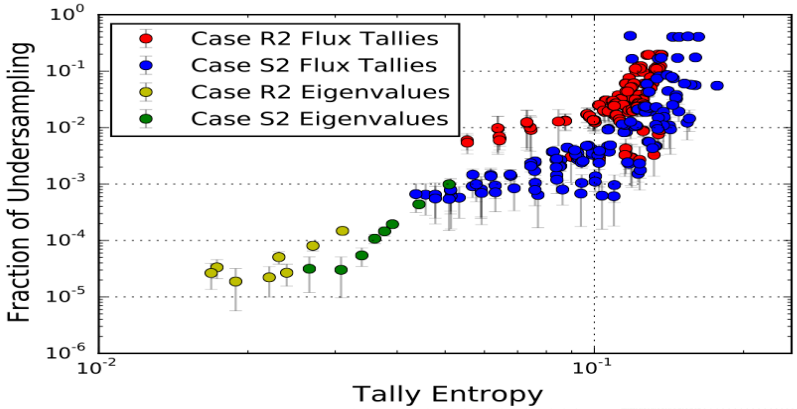


Undersampling in Case S2 pin flux tallies [Perfetti and Rearden 2014]

Background

- In 2014, several statistical metrics were investigated for their potential to predict undersampling biases in the EGAMCT benchmark problems.
- Several metrics were found to potentially predict both the onset and magnitude of undersampling biases.



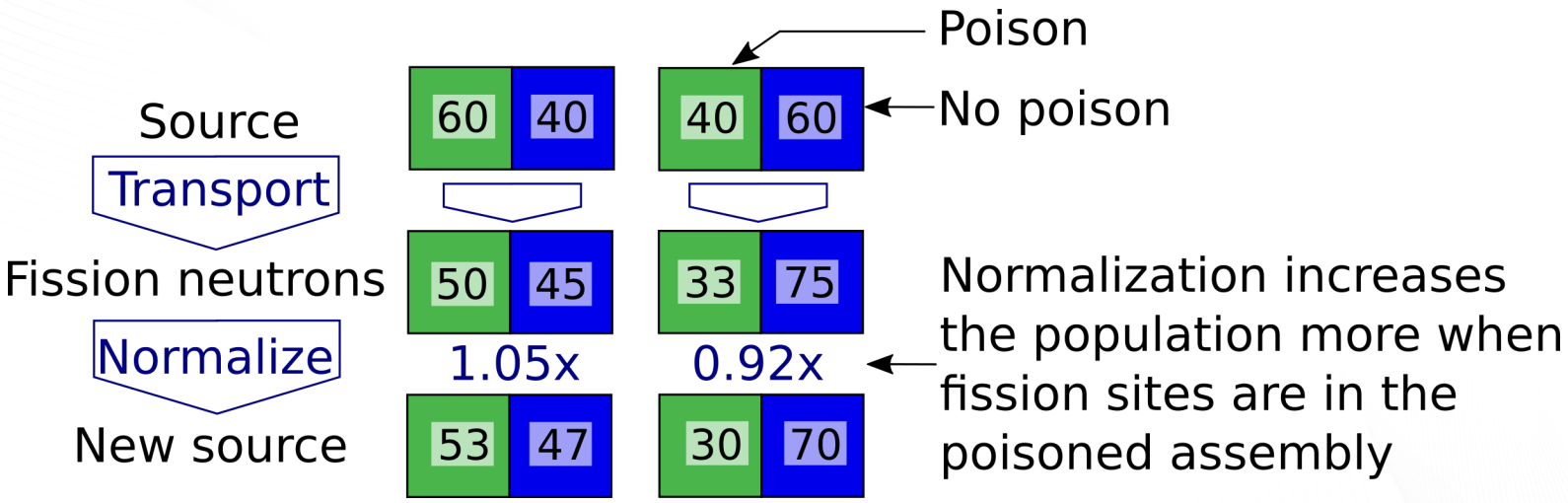


Magnitude of undersampling biases versus the number of tally scores per generation (left) and tally entropy (right)
[Perfetti and Rearden 2015]

Overview

- Brissenden and Garlick's theory
- New theory
- Demonstration problems and results
  - Godiva
  - Pin Cell
  - C5G7
- Comparison with alternative metrics
- Ongoing challenges

Brissenden & Garlick 1986
Theory



Brissenden & Garlick 1986
Derived Correction

Weight correction →

$$\alpha_L^{(g)} \equiv \prod_{g'=g-L}^{g-1} k^{(g')}$$

Corrected k →

$$k_L = \frac{\sum_g \alpha_L^{(g)} k^{(g)}}{\sum_g \alpha_L^{(g)}}$$

Generalization of the BG Correction

Any Boltzmann tallies can be corrected

Same weight correction →

$$\alpha_L^{(g)} \equiv \prod_{g'=g-L}^{g-1} k^{(g')}$$

Corrected tally →

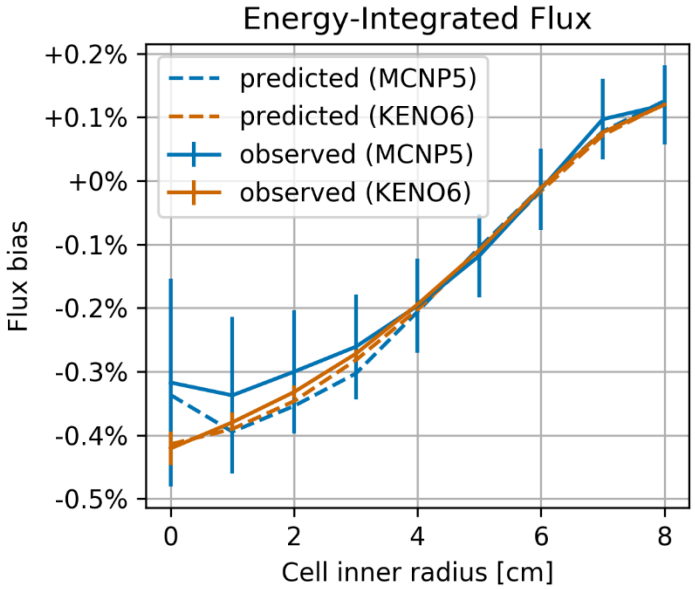
$$T_L = \frac{\sum_g \alpha_L^{(g)} T^{(g)}}{\sum_g \alpha_L^{(g)}}$$

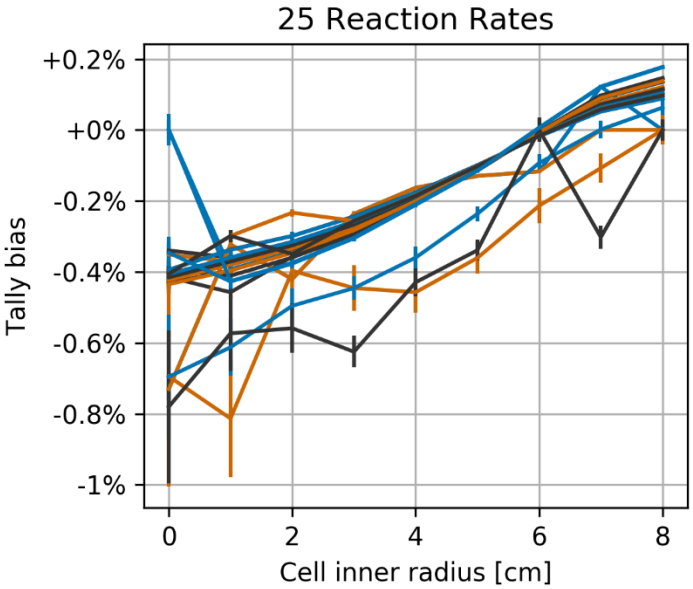
Generalized correction formula

Using the correction to estimate bias

- Create an energy-integrated mesh tally over the region of interest
- Dump $k^{(g)}$ and $T^{(g)}$ every generation
- Calculate T_L in post-processing
- Subtract T_L from T_0 → "predicted" bias
- Compare T_0 to results with large NPG → "observed" bias

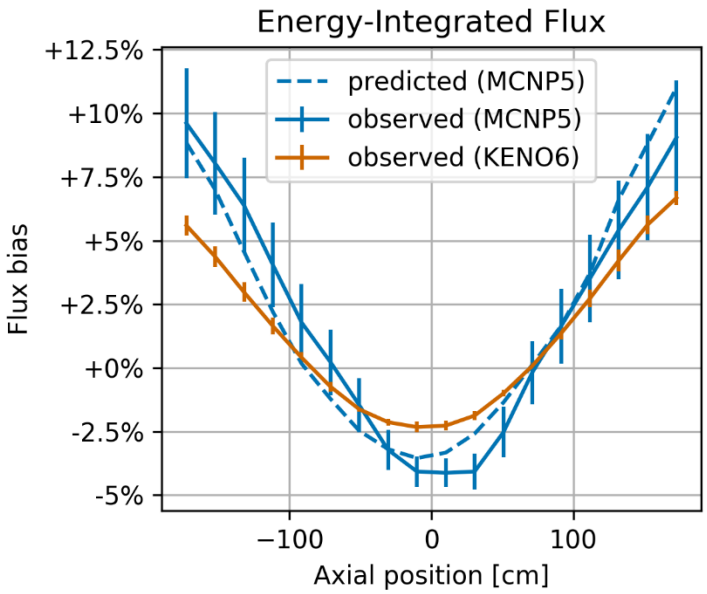
Godiva Results

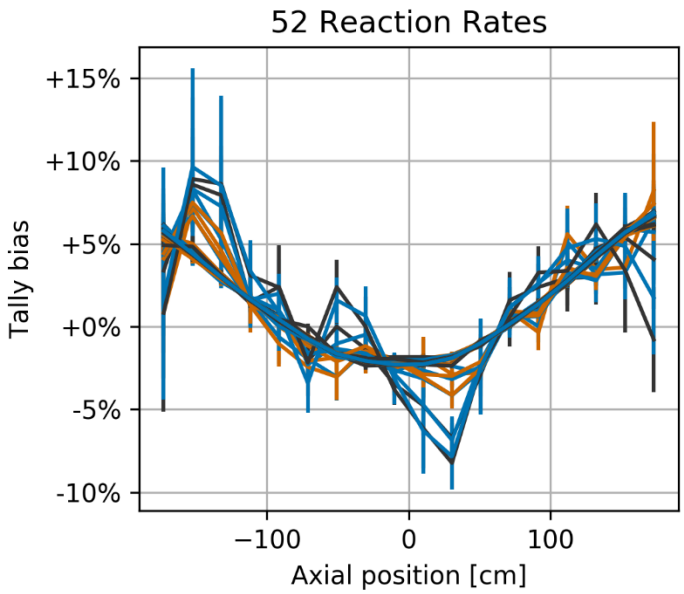




# of correction terms: *L* = 20

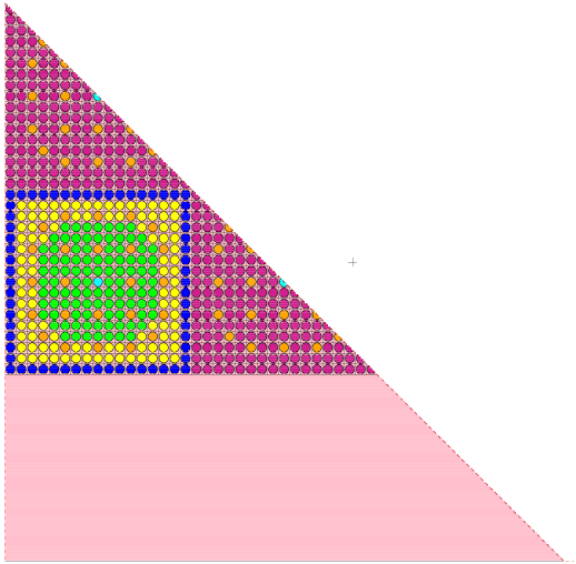
Pin Cell Results



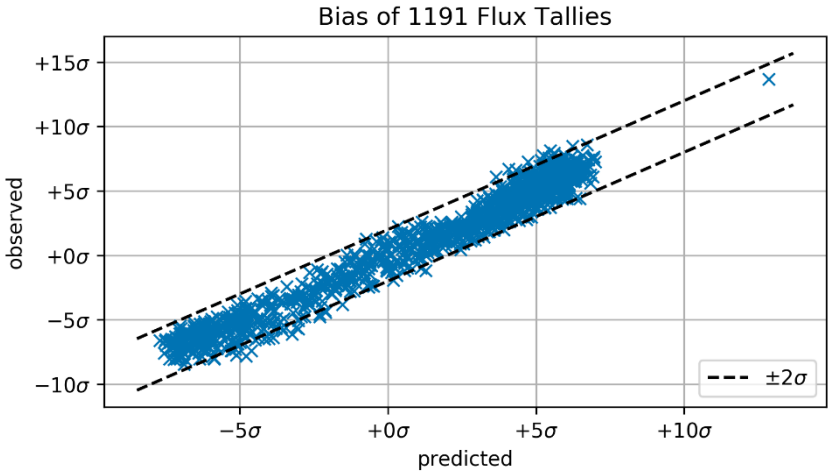


# of correction terms: *L* = 100

C5G7 Results



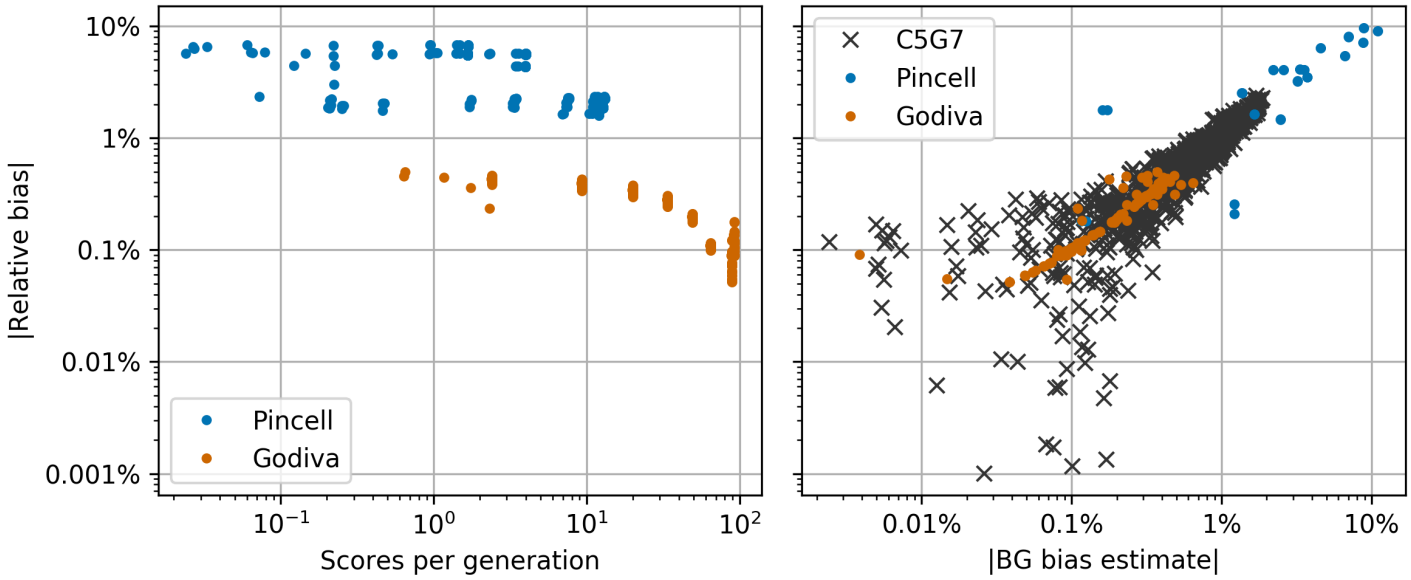
2D model from corephysics.com



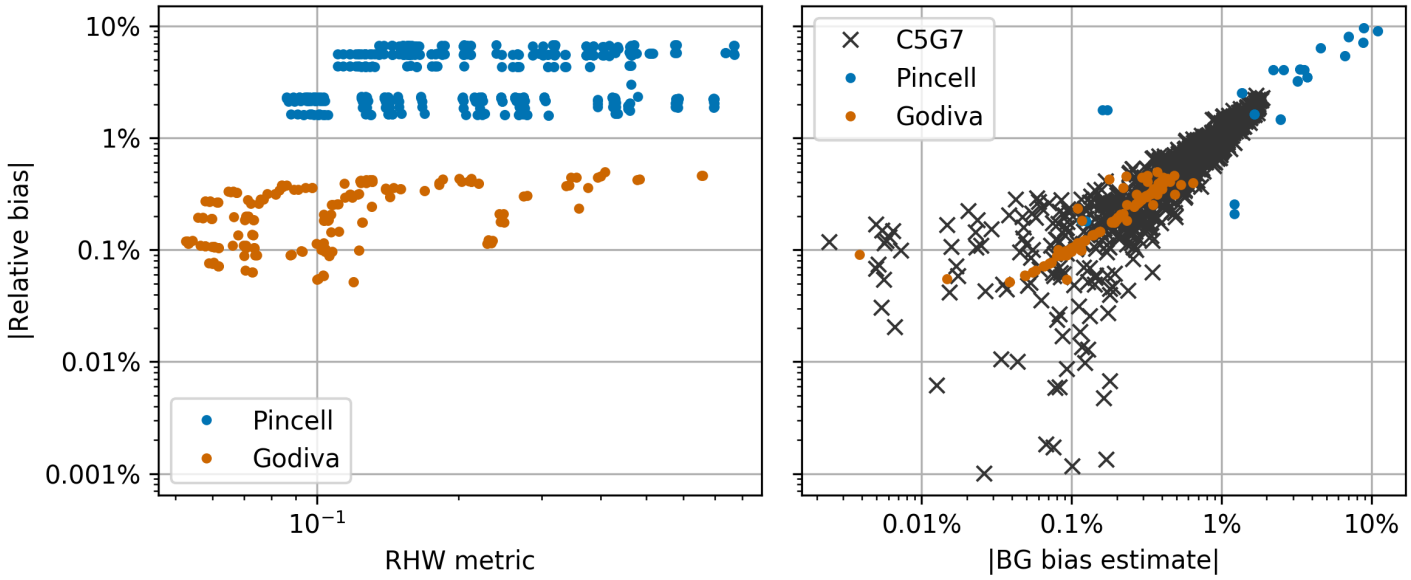
Most bias observations are within 2 standard deviations of predictions

# of correction terms: L = 10

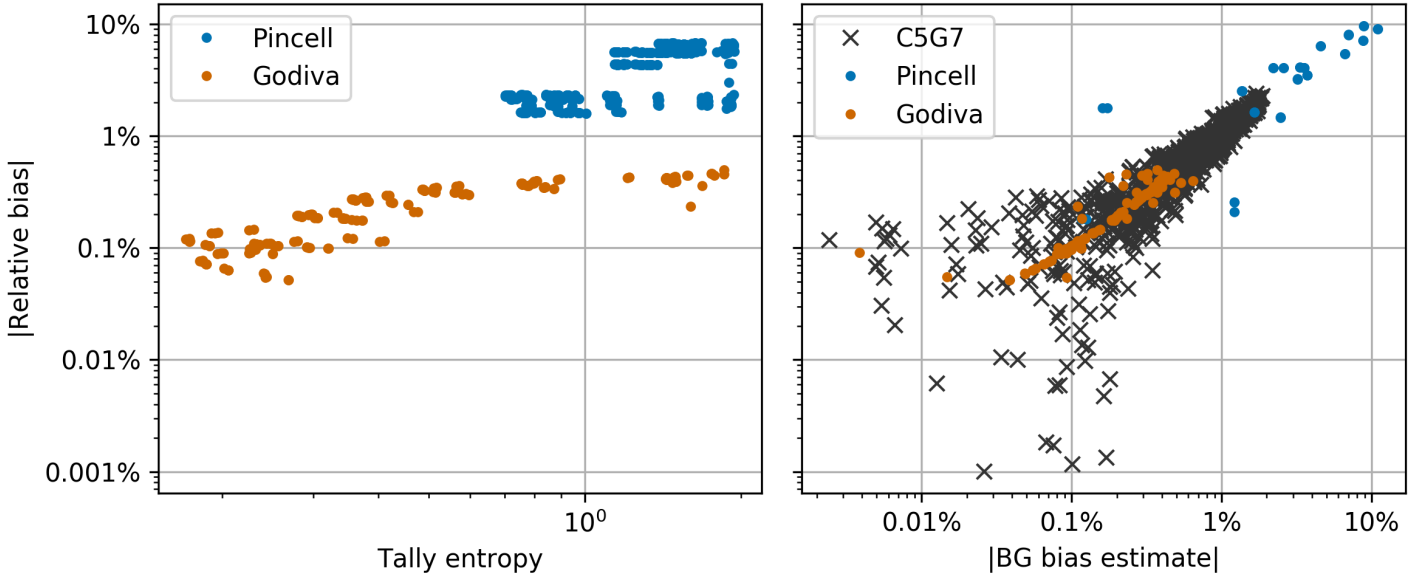
Comparison with Other Metrics
Scores per Generation



Comparison with Other Metrics
Heidelberger–Welch Relative Half-Width Metric



Comparison with Other Metrics
Tally Entropy



Summary

Progress

- Demonstrated that the BG correction can predict bias for *k* and tallies.
- Demonstrated that the relative bias is independent of reaction weighting.

Ongoing Work

- Demonstration with energy-binned tallies.
- Demonstration on the EGAMCT benchmark problem.
- Methodology to select *L.*
  - Tradeoff between bias (*L* too small) and noise (*L* too large).

Questions?

Please contact:

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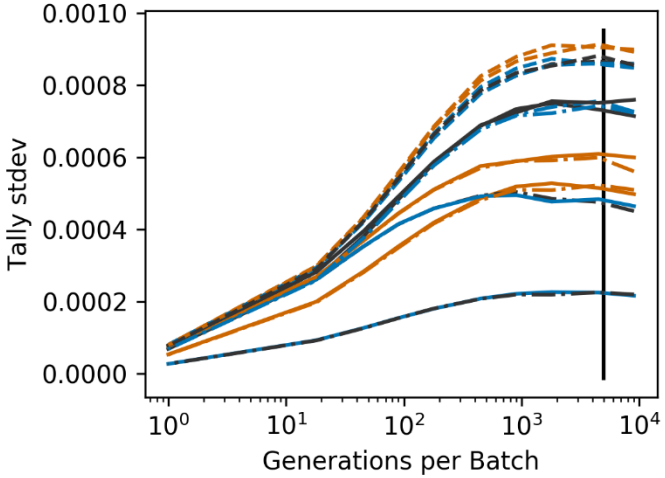
Miscellaneous

Typical Procedure

- Simulate a “naïve” case with NPG=10^2 and a “reference” case with NPG=10^5. Both cases simulate 10^8 total histories (10^7 inactive).
- Estimate uncertainty using batch statistics. Multiple generations per batch---see next slide.
- “Observed” bias is naïve minus reference.
- “Predicted” bias is calculated from the naïve case.
  - Use the smallest L such that $T_L \sim T_{2L}$.

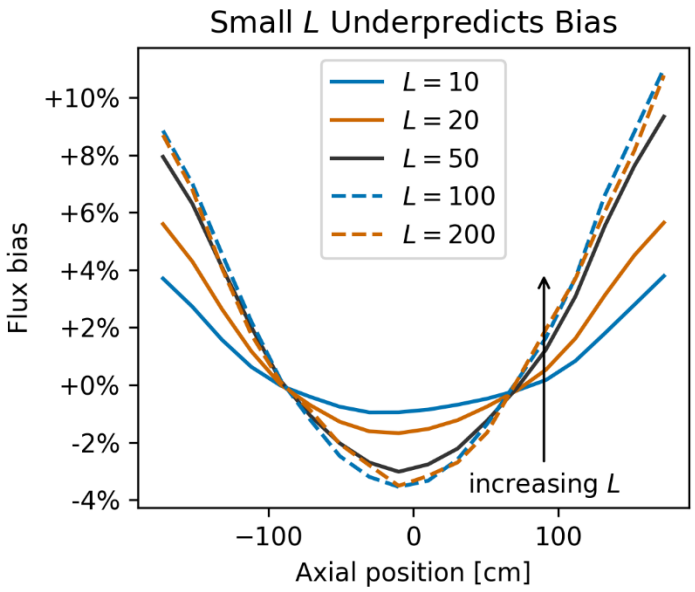
Batch-size Selection

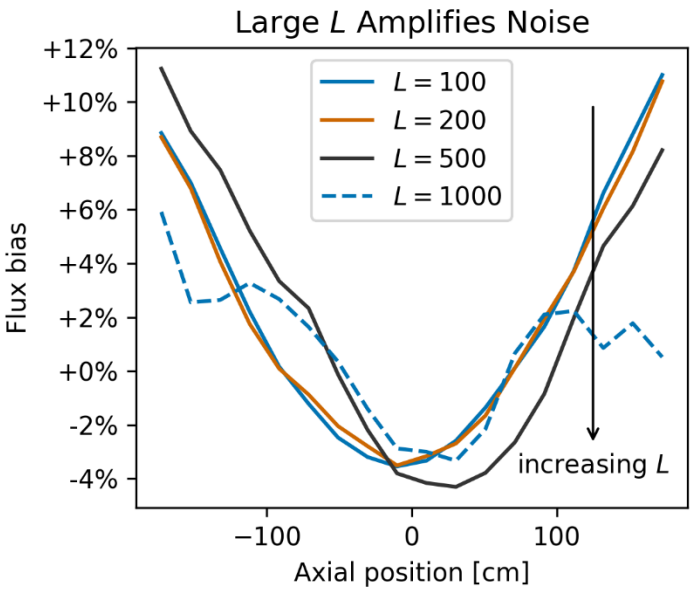


Correlations among generations require multi-generation batch statistics.

Use the smallest possible batches that appear to give consistent precision estimates (black vertical line).

Effect of *L*
Pin Cell Problem





Proposed Methodology to Select *L*

- Tradeoff between bias (*L* too small) and noise (*L* too large).
- Methodology:
  - On an energy-integrated coarse mesh, tally T_0, T_{100}, and T_{200}
  - Bias in all tallies is comparable to bias in T_0.
  - Compare T_0 to T_{100} to estimate the tally bias
  - Compare T_{100} to T_{200} to assess whether T_{100} is biased