

# Diagnosing Undersampling in Monte Carlo Eigenvalue and Flux Tally Estimates

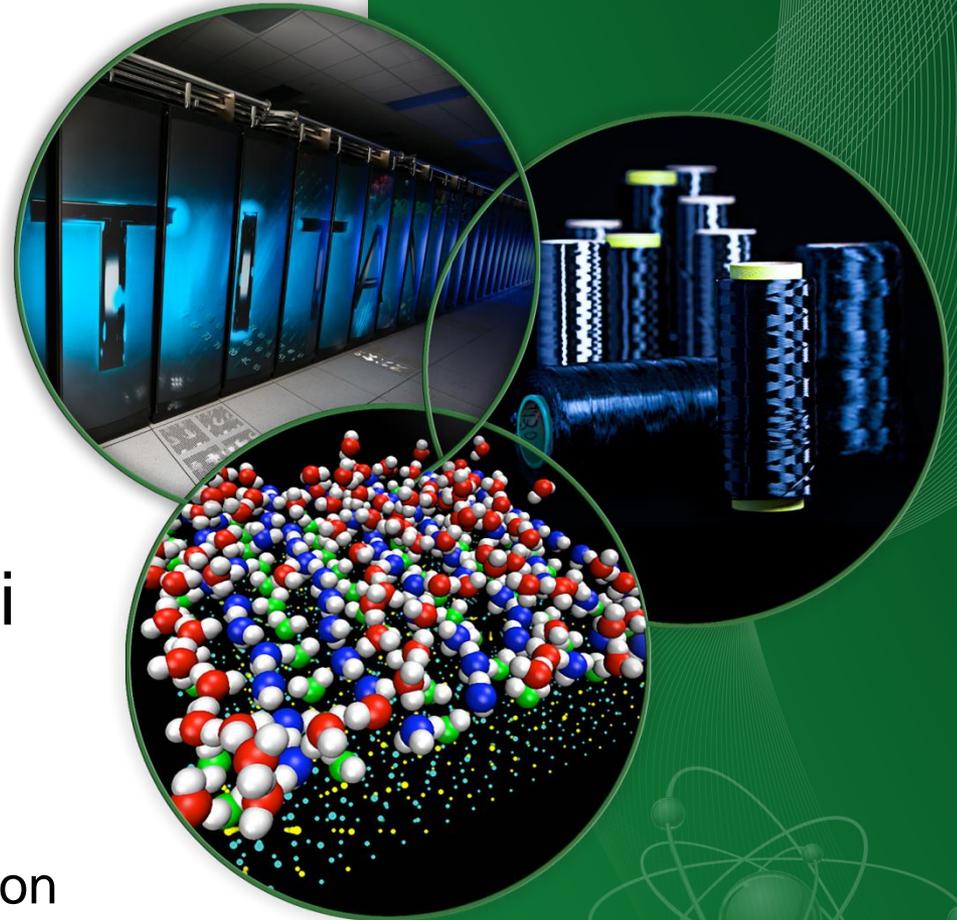
Dr. Christopher M. Perfetti

Dr. Bradley T. Rearden

Radiation Transport Group

Reactor and Nuclear Systems Division

Oak Ridge National Laboratory

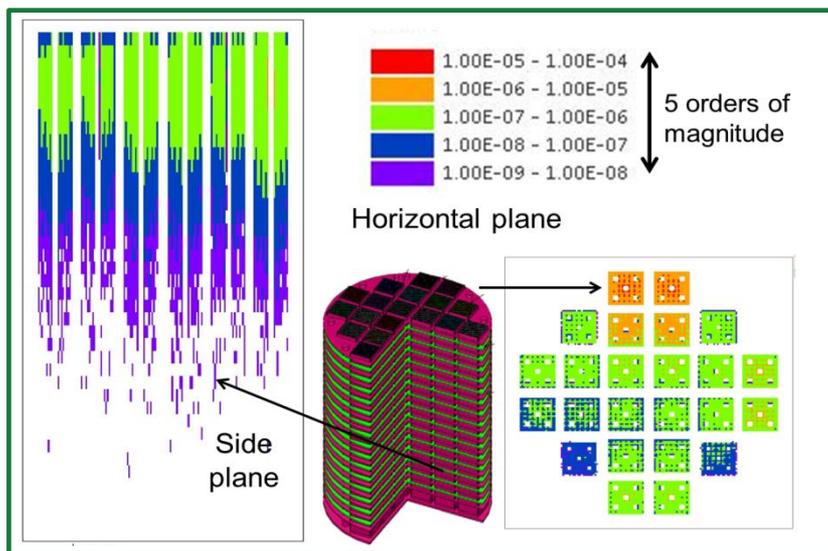


ORNL is managed by UT-Battelle  
for the US Department of Energy

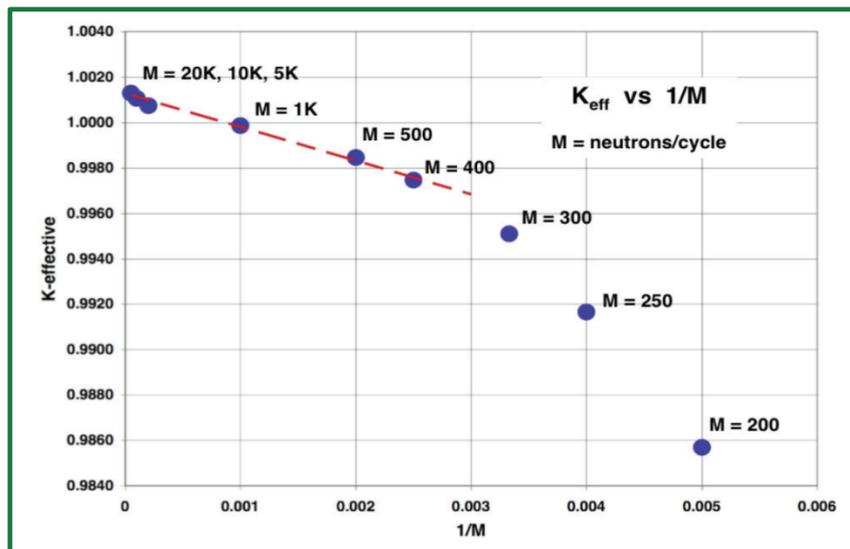
 OAK RIDGE  
National Laboratory

# 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.



(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

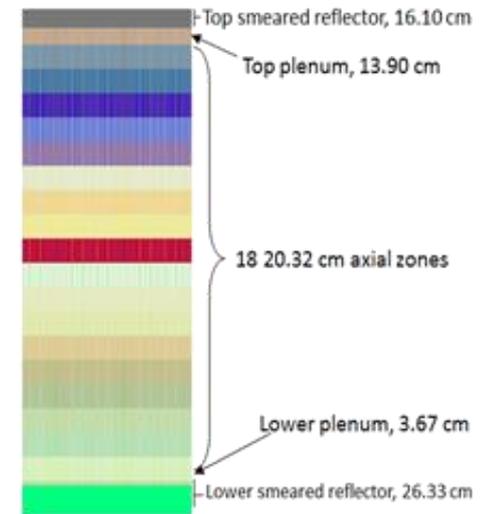
## Three Benchmark Cases:

R1 = 2D Core

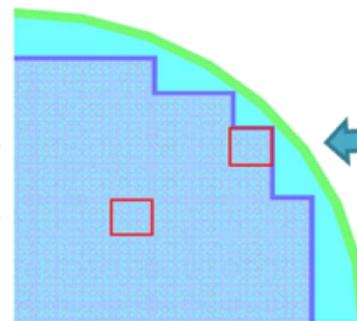
R2 = 3D, Infinitely Reflected Assembly

R3 = 3D Core

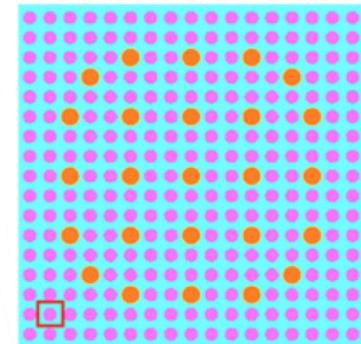
- Fuel temperature varies with axial location
- Isotopics corresponding to 20 GWd/MTU fuel



Assembly Axial Slices



Assembly Locations



Fuel Pin Location in each Assembly

[Perfetti and Rearden, 2014]

# EGAMCT Benchmark Problems: Shipping Cask Cases

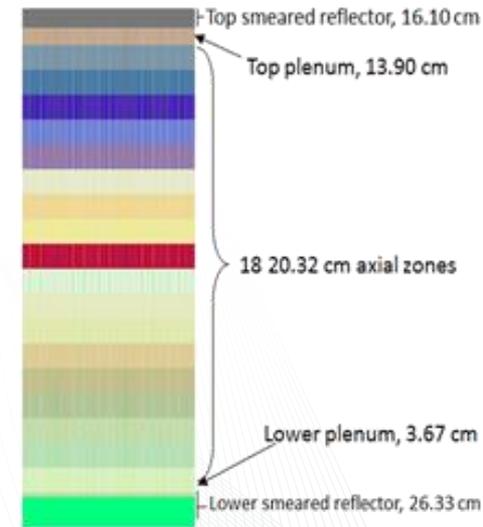
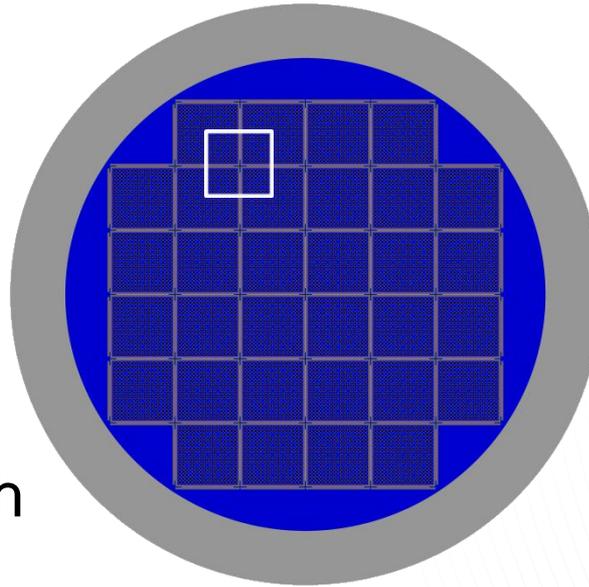
## Three Benchmark Cases:

**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

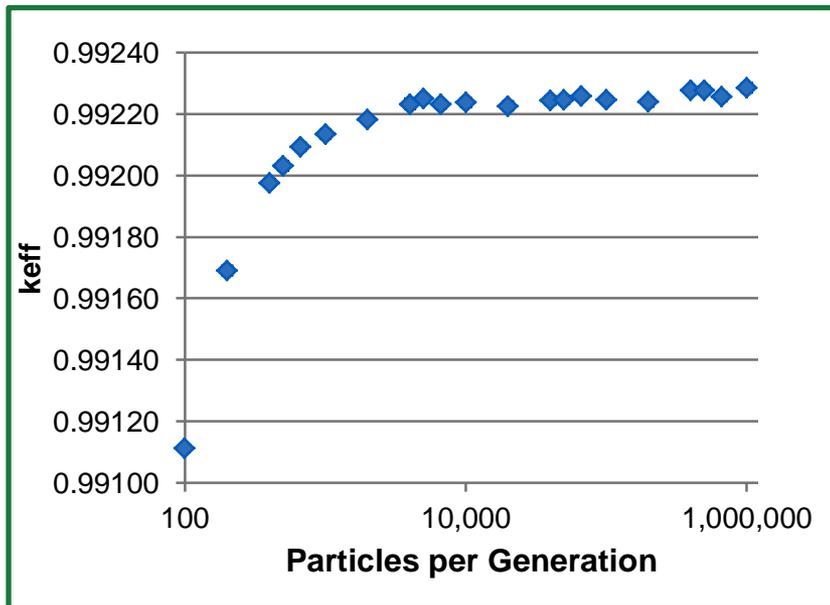


Assembly Axial Slices

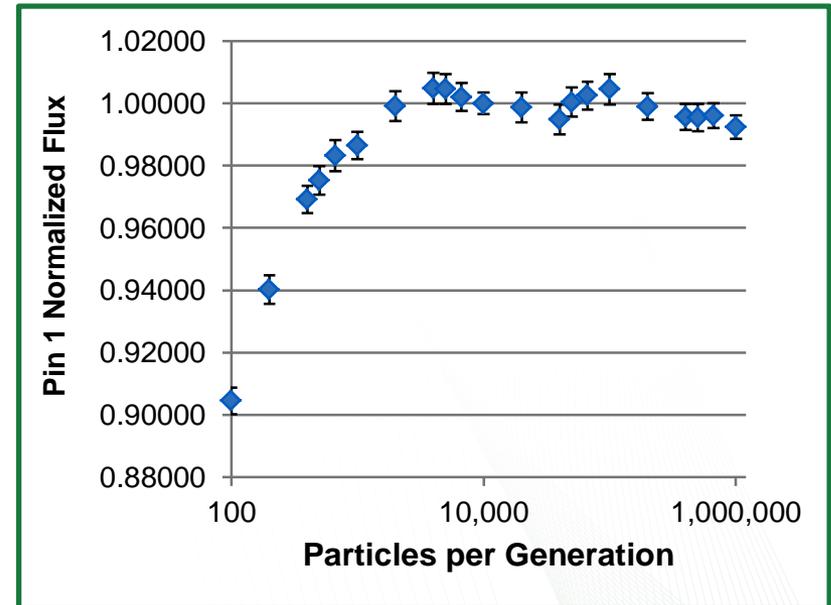
[Perfetti and Rearden, 2014]

# Undersampling Biases

- In 2014 Perfetti and Rearden observed significant undersampling biases 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.

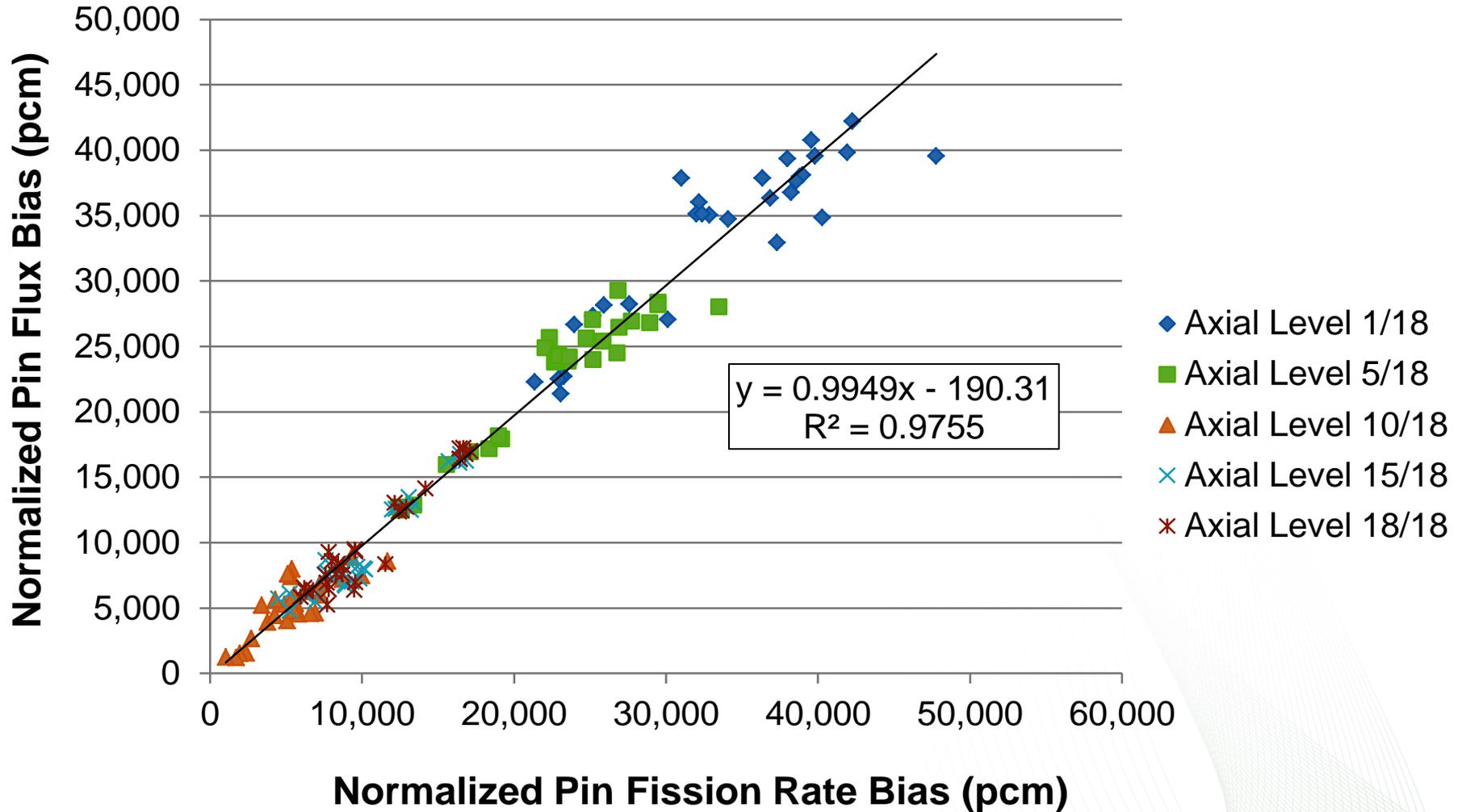


**Undersampling in Case R1 Eigenvalues  
(Perfetti and Rearden 2014)**



**Undersampling in Case S2 Pin Flux Tallies  
(Perfetti and Rearden 2014)**

# Undersampling Biases: R3 Case



# Predicting Undersampling Biases

- This study investigates potential metrics for detecting undersampling by applying several Markov chain convergence metrics to previous EGAMCT results.
- The overall goal of this work is to identify metrics for predicting the onset and magnitude of undersampling biases.

# Metrics Examined in This Study

- Contributing Particles per Generation
- Heidelberger–Welch RHW
- The Geweke Z-Score
- Gelman–Rubin Diagnostics
- Tally Entropy

# Metric Evaluation

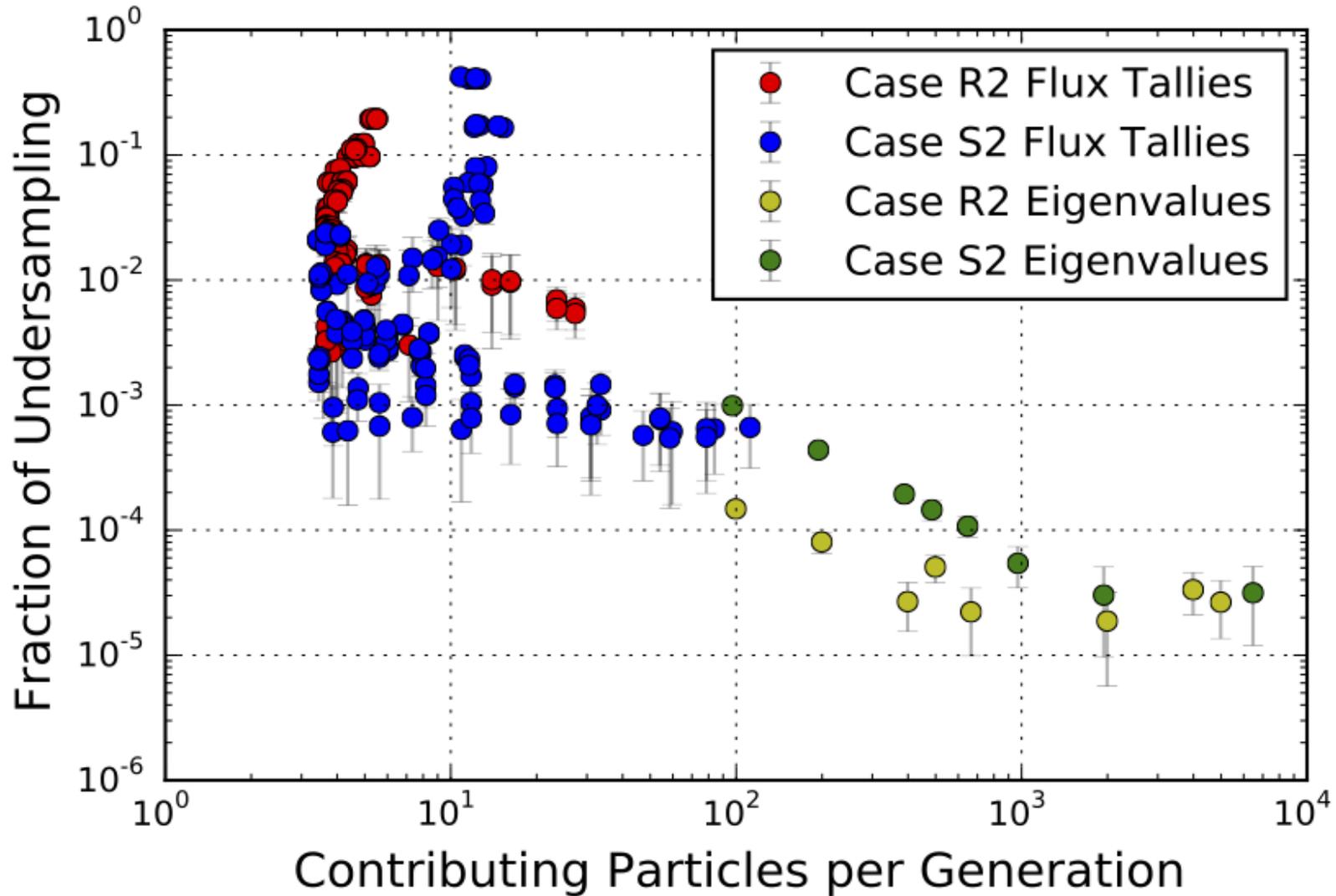
- The goal of this study is to find metrics that can predict the occurrence of undersampling biases. Ideally, these metrics will also correlate strongly to the magnitude of the undersampling bias.
- The **Fraction of Undersampling** was used to measure the magnitude of the undersampling biases, where:

$$\text{Fraction of Undersampling} \equiv \frac{|\text{Biased Score} - \text{Unbiased Score}|}{\text{Unbiased Score}}$$

# Contributing Particles per Generation

- This metric simply counts the average number of particles that contribute nonzero scores to an ROI within each generation.

# Contributing Particles per Generation Results

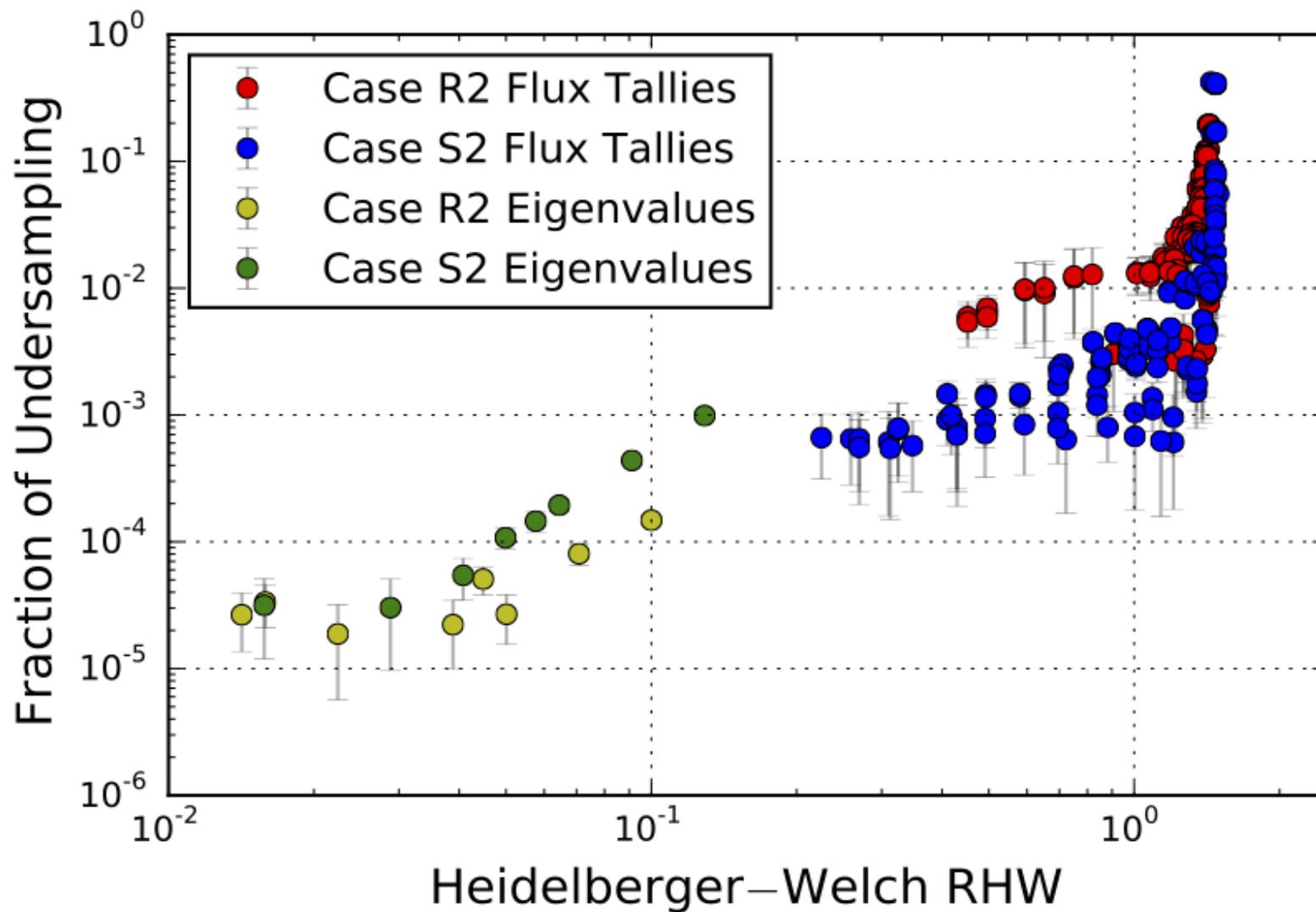


# Heidelberger–Welch Relative Half-Width

- The Heidelberger–Welch Relative Half-Width (RHW) test assesses convergence by determining if the samples within a Markov chain vary significantly outside the confidence interval ( $\alpha$ ) of that chain.

$$RHW = \frac{Z_{(1-\alpha/2)} \sqrt{\hat{S}_n/n}}{\theta_n}$$

# Heidelberger–Welch RHW Results



# Heidelberg–Welch RHW Results

- In general, large RHW values were a good indicator of undersampling.
- Undersampling was observed for all nonzero RHW values. Tallies with smaller RHW values tended to show less undersampling.

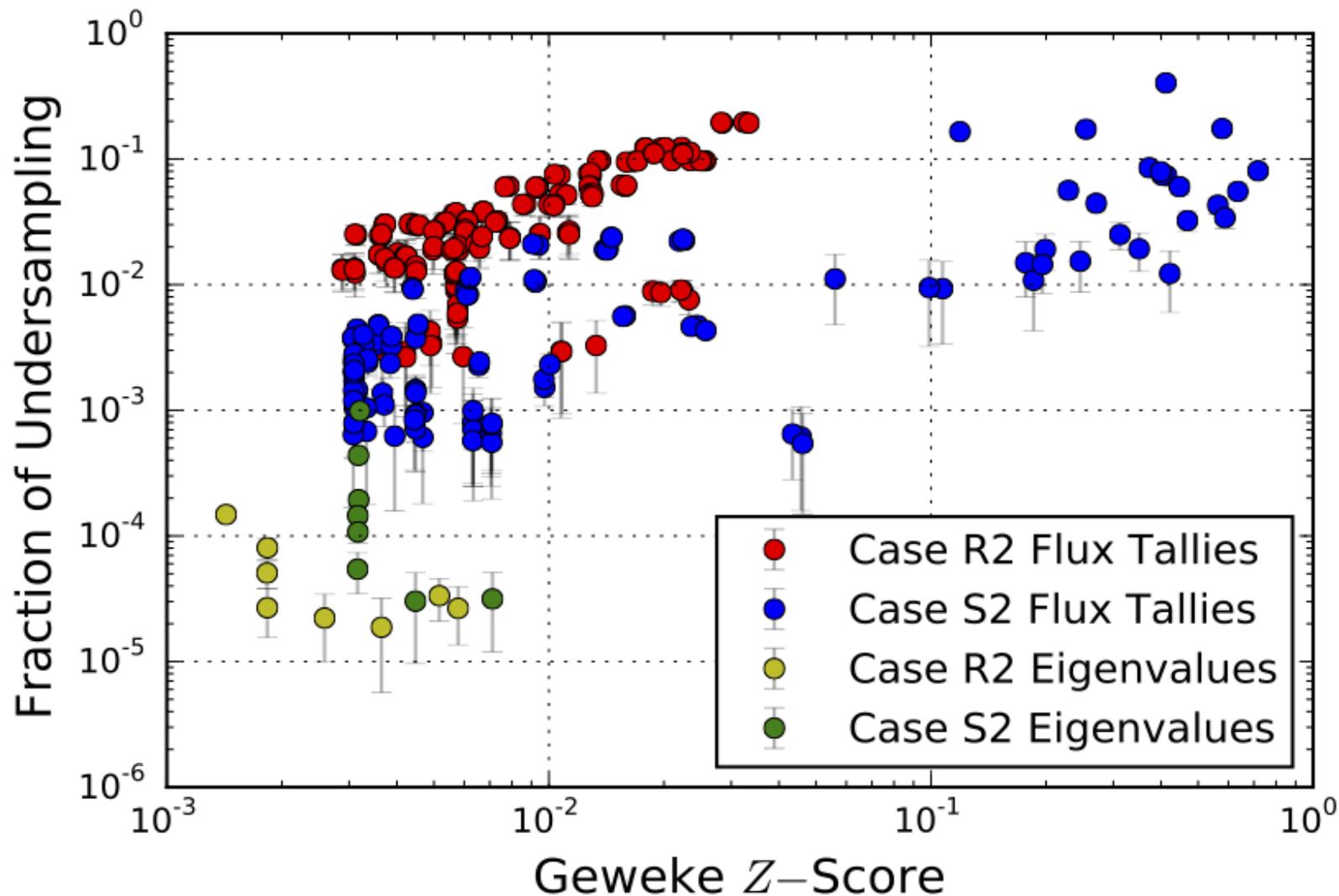
# Geweke Diagnostics

- The Geweke Z-Score tests for convergence by comparing the average contributions of tallies in the first and second halves of a Markov chain.

$$Z = \frac{\theta_1 - \theta_2}{\sqrt{\frac{\hat{S}_{n_1}}{n_1} + \frac{\hat{S}_{n_2}}{n_2}}}$$

- In this application, the Markov chain is considered to be the contribution of individual particles to a ROI within a single generation.

# Geweke Diagnostics Results



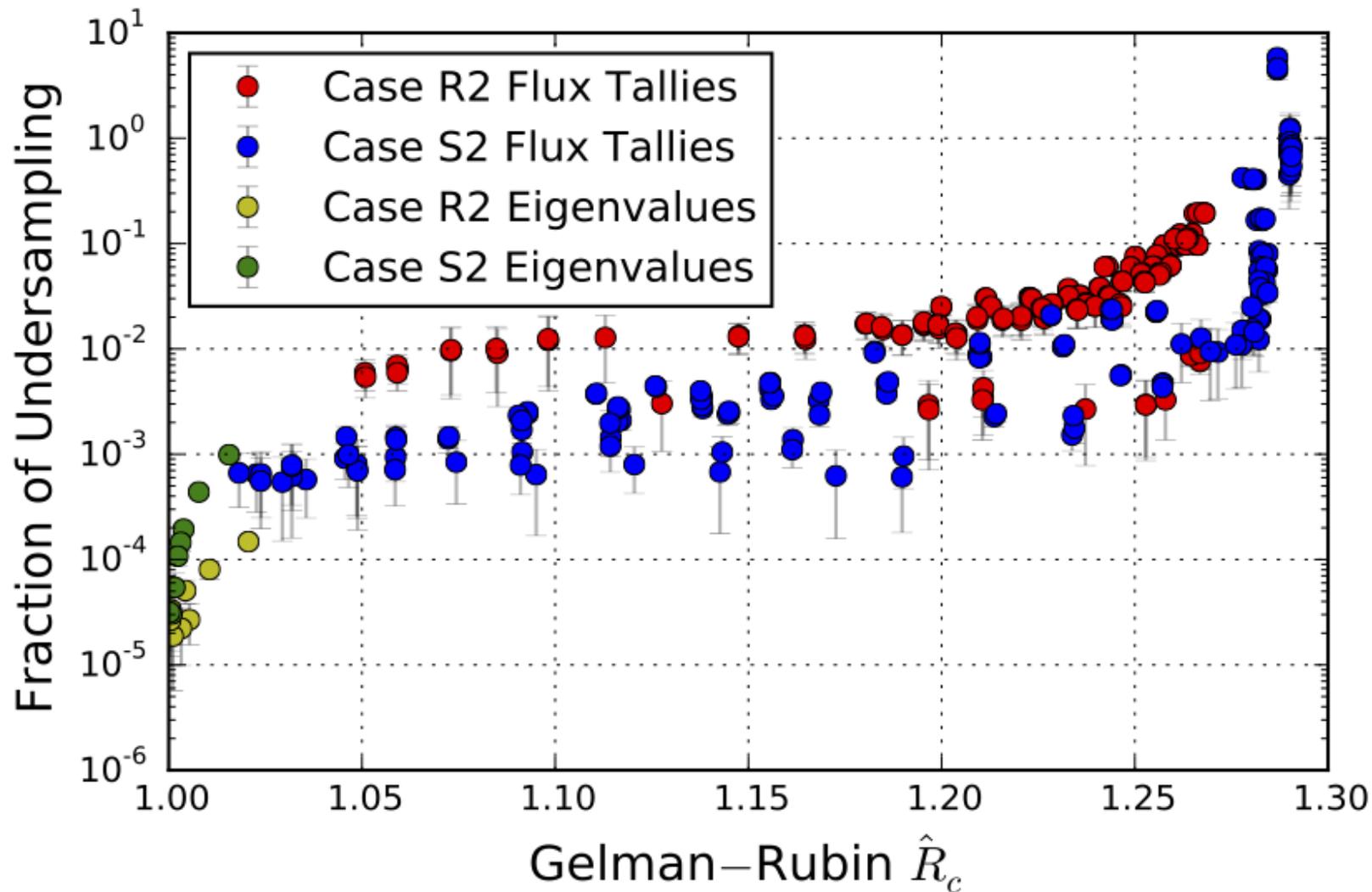
# Geweke Diagnostics Results

- The Geweke Z-Score did not effectively predict the onset of undersampling.

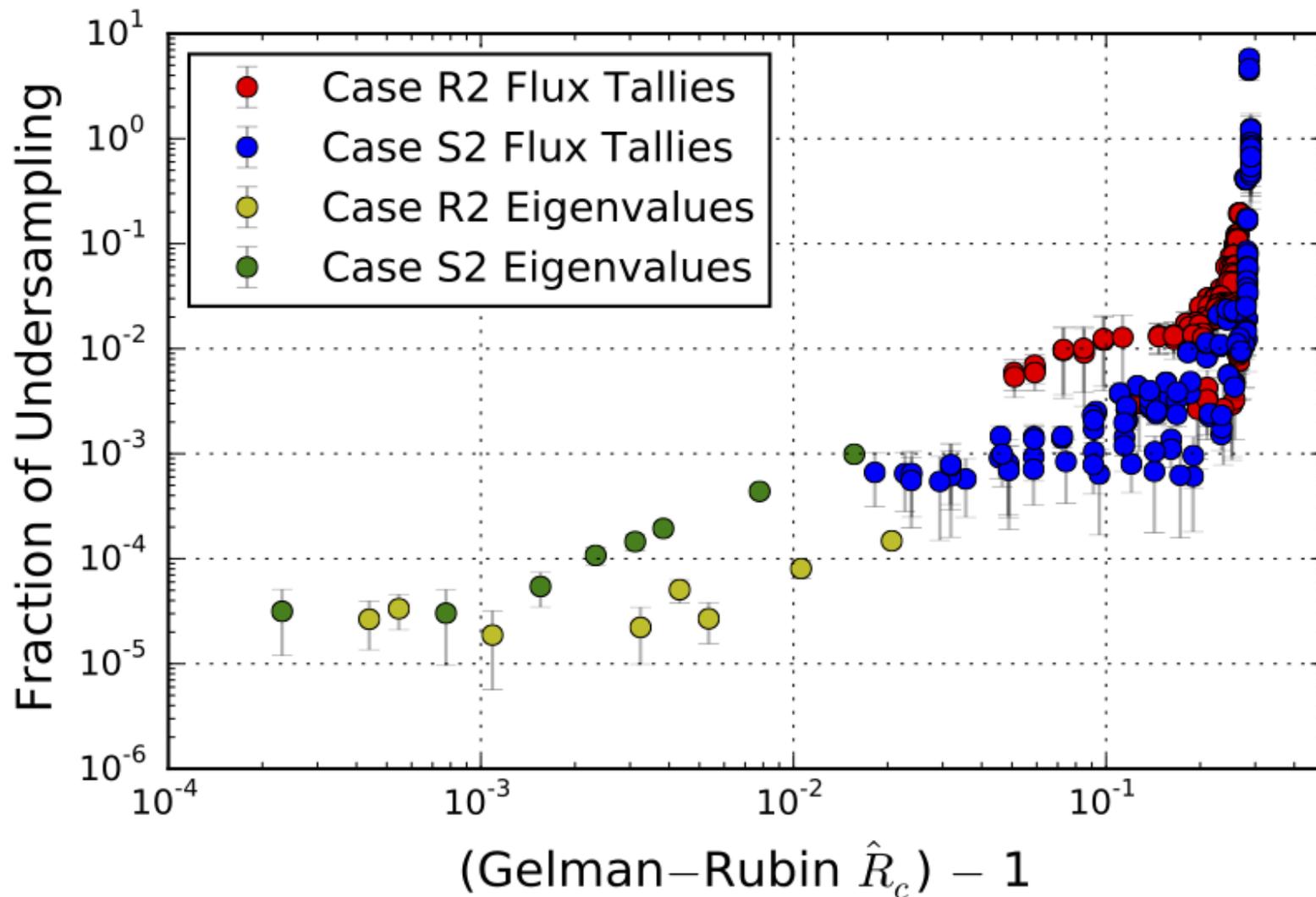
# Gelman–Rubin Diagnostics

- This metric separates events within a Markov chain (i.e., tally scores of particles within a single generation) into several subchains and assesses convergence by comparing the ROI variance within and between the subchains.
- Gelman–Rubin Diagnostics are popular metrics for assessing the convergence of Markov chains.

# Gelman–Rubin Diagnostics Results



# Gelman–Rubin Diagnostics Results



# Gelman–Rubin Diagnostics Results

- Gelman–Rubin Diagnostics were observed to effectively predict the onset of undersampling.
- Unlike the Heidelberger–Welch RHW and Tally Entropy metrics, the Gelman–Rubin  $\hat{R}_c$  metrics effectively predicted undersampling for very poorly converged tallies.

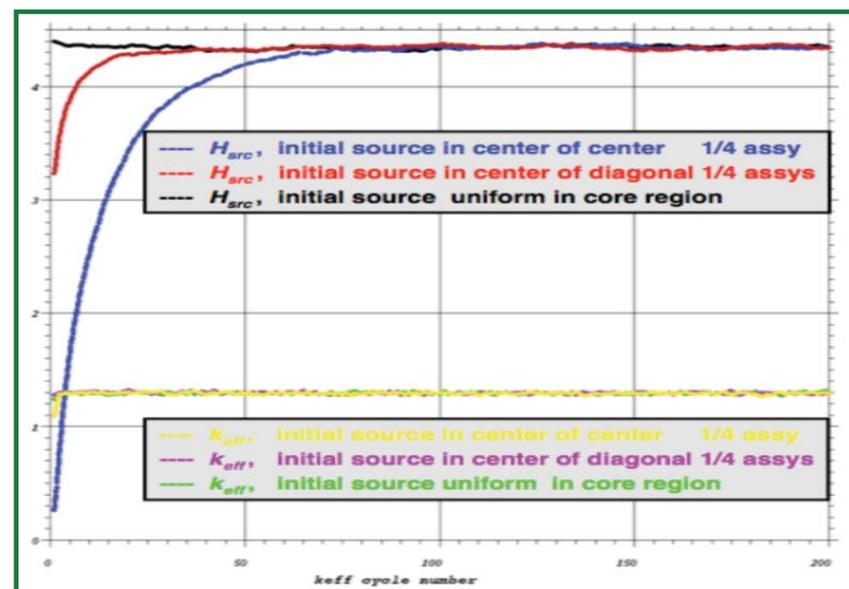
# Tally Entropy – A New Diagnostic

- Shannon Entropy is a concept from Information Theory that measures the amount of information contained in messages in a data stream.

$$H = - \sum_n^N p_n \ln(p_n)$$

$$\max(H) = \ln(N)$$

- Recently, Brown and Ueki employed Shannon Entropy to diagnose convergence of the fission source in eigenvalue calculations.



Convergence of Shannon Entropy  
in a 2D full core PWR calculation

(Brown 2011)

# Tally Entropy – A New Diagnostic

- Undersampling occurs when some particles contribute too much information to tally estimates and other particles contribute too little information. This behavior minimizes the “entropy” of tally calculations.
- The “tally entropy” of tally  $i$  for particles in generation  $j$  was defined by calculating the Shannon Entropy of the fractional contribution of each particle,  $p_x$ , to tally  $i$ .

$$p_x = \frac{\textit{Tally Score of Particle } x}{\textit{Sum of all Tally Scores in Gen. } j}$$

$$H_{i,j} = \sum_{\textit{Particle } x}^{\textit{All Particles in Gen. } j} -p_x \ln(p_x)$$

# Tally Entropy – A New Diagnostic

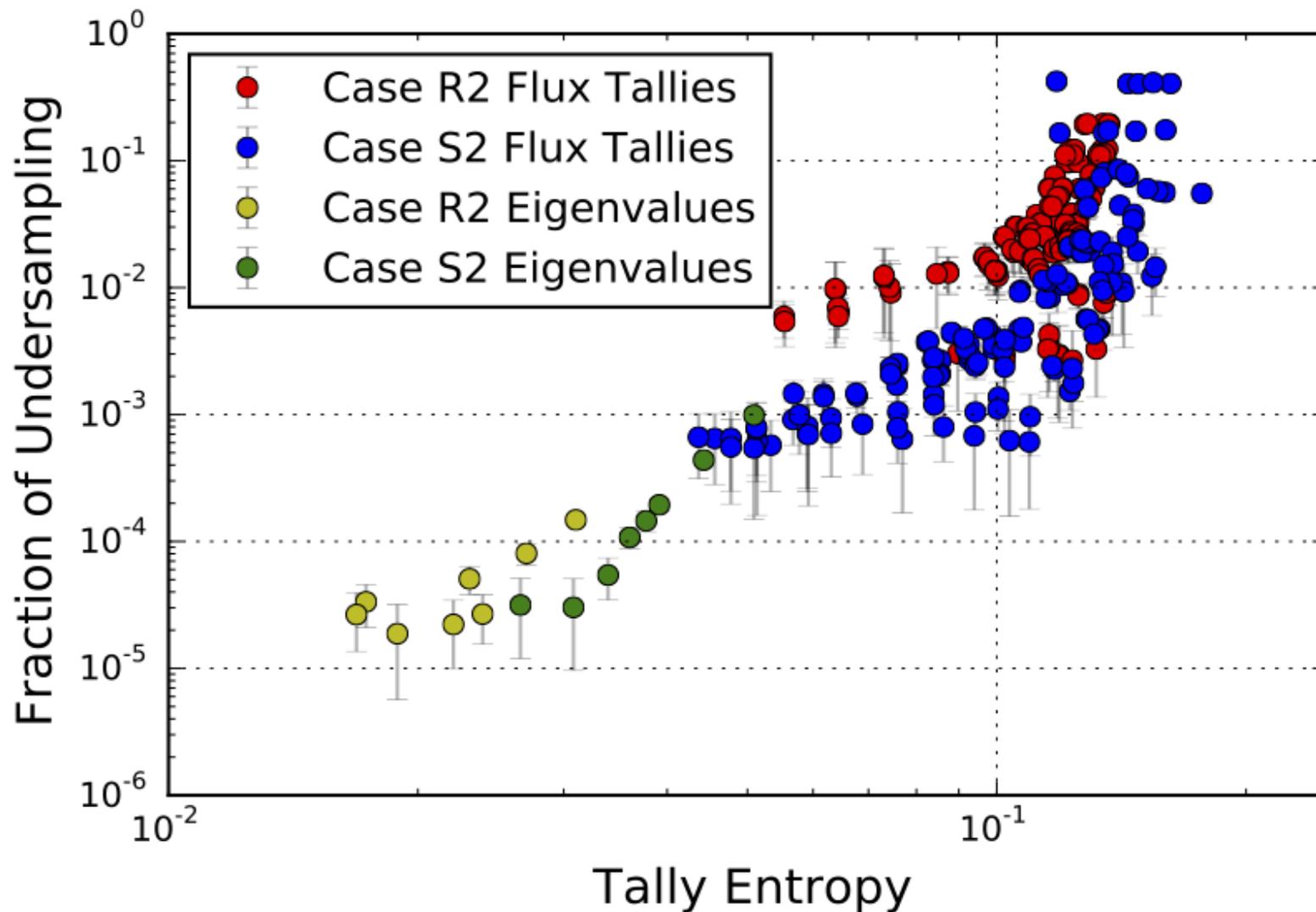
- The tally entropy approaches  $\ln(N)$  as:
  - the number of tally scores in a generation,  $N$ , approaches infinity, and
  - the tallies make uniform contributions to the ROI.

**These are ideal conditions for preventing undersampling.**

- A new test statistic was developed by examining the fractional difference between the entropy of a tally,  $H_i$ , and its limit of  $\ln(N_i)$ :

$$\text{Tally Entropy} \equiv \frac{(\ln(N_i) - H_i)}{\ln(N_i)}$$

# Tally Entropy Results



# Tally Entropy Results

- Like the Heidelberger–Welch RHW and Gelman–Rubin metrics, tally entropy shows promising potential for predicting undersampling.
- Tally entropy calculations produced poor results for extremely undersampled tallies.

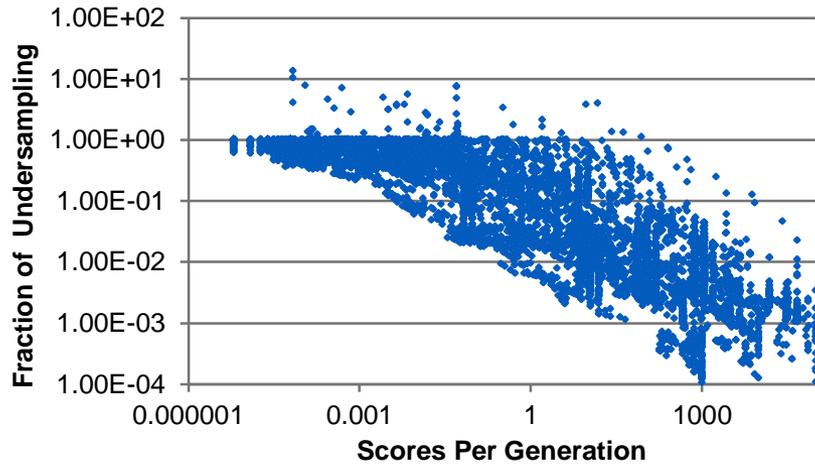
# Conclusions

- The Heidelberger–Welch RHW, Gelman–Rubin, and Tally Entropy diagnostics were able to predict the onset of undersampling.
- The Contributing Particles per Generation metric was able to somewhat predict undersampling, and the Geweke Z-Score was a poor indicator of undersampling.
- Undersampling was observed for both eigenvalue and flux tally calculations. Undersampling was observed for even small/optimal values of the convergence metrics, suggesting that undersampling may be present (perhaps in miniscule amounts) in all Monte Carlo simulations.

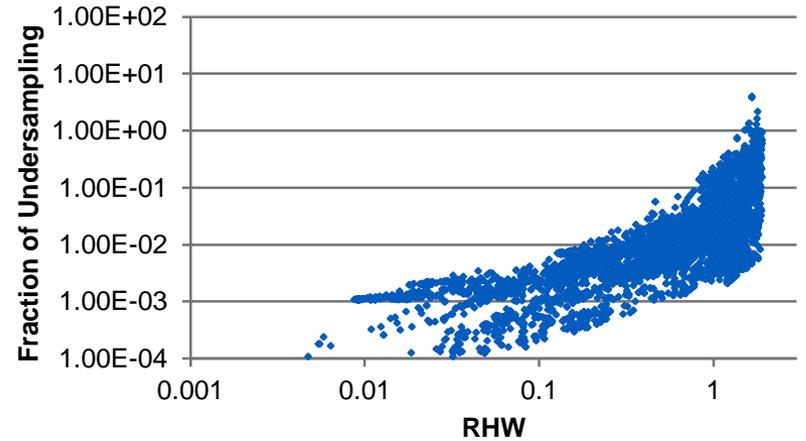
# Future Recommendations

- Apply these convergence diagnostics to a wider range of problems and ROIs (multigroup fluxes, reaction rates, etc.) and determine if a **problem-independent** metric exists that can predict the onset **and magnitude** of undersampling.
- Develop approaches (hybrid methods, FW-CADIS, etc.) for minimizing these metrics and mitigating the impact of undersampling.

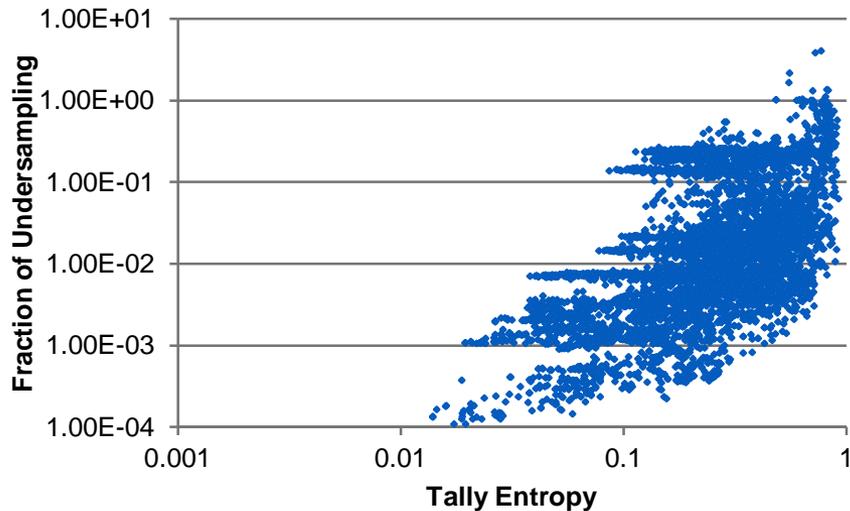
# Future Recommendations



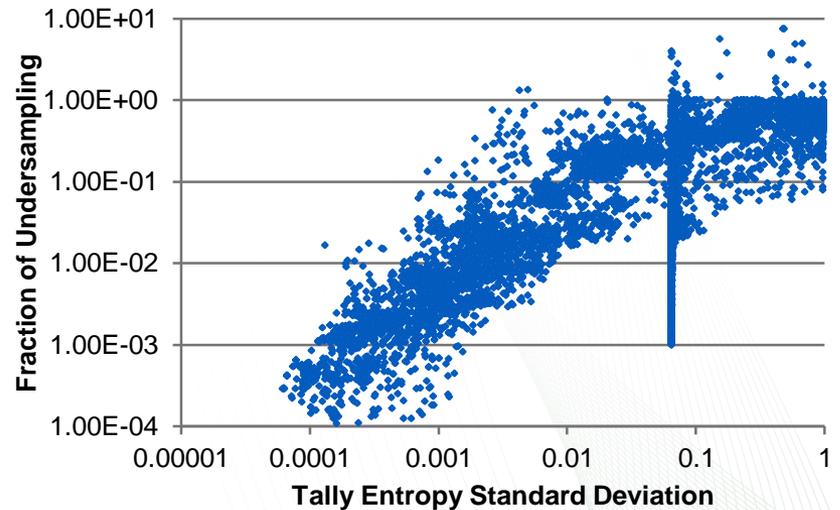
## 1. Scores per Generation



## 2. Filtered RHW



## 3. Filtered Tally Entropy



## 4. Tally Entropy St. Dev.

# Future Recommendations

- To ensure that undersampling has an impact of less than 1% on the accuracy of Monte Carlo flux tallies, it is recommended that:
  - Heidelberg–Welch  $RHW \leq 0.50$
  - Gelman–Rubin  $\hat{R}_c \leq 1.05$
  - Tally Entropy  $\leq 5\%$

# Questions???

Please contact:

Chris Perfetti  
perfetticm@ornl.gov