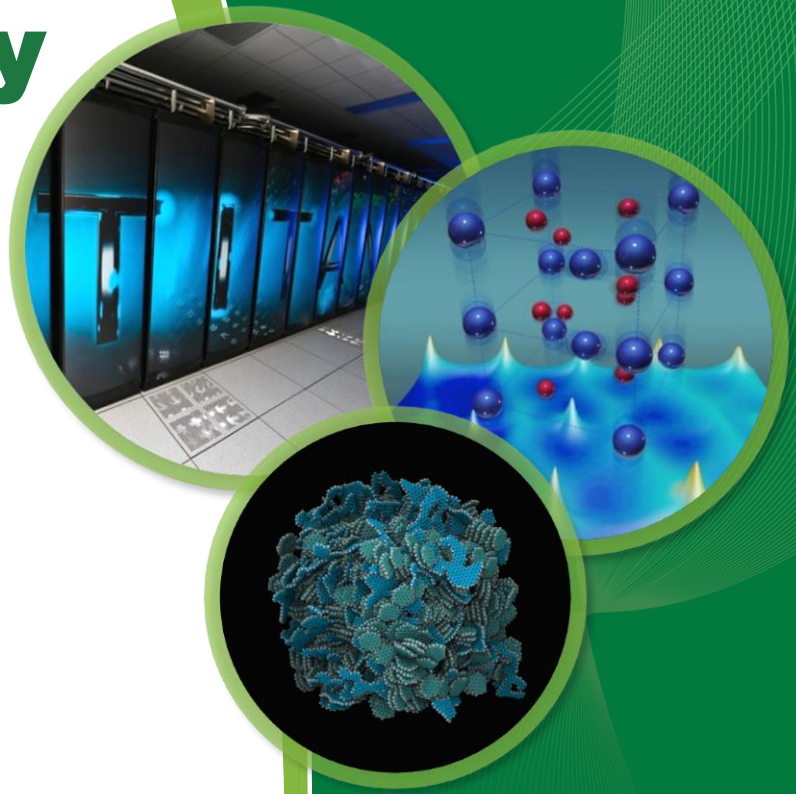
SCALE Continuous-Energy Undersampling Bias and Metric Results



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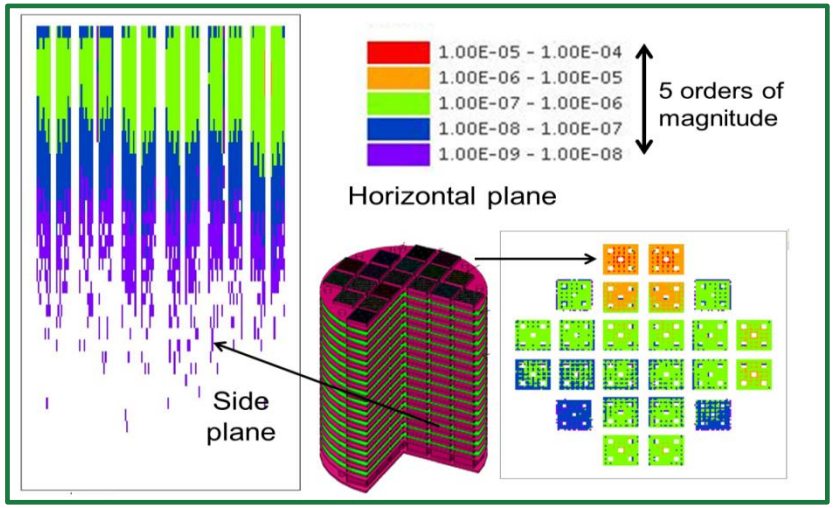
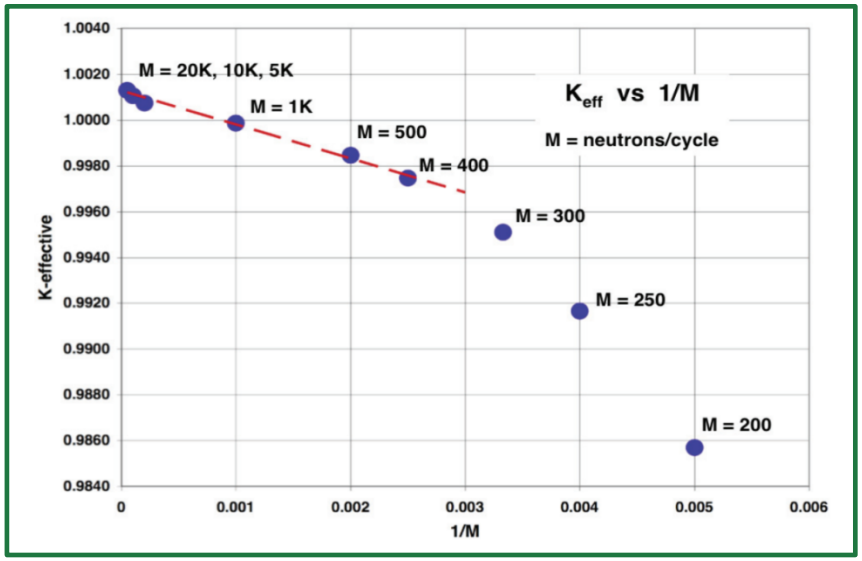
Introduction

- 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.

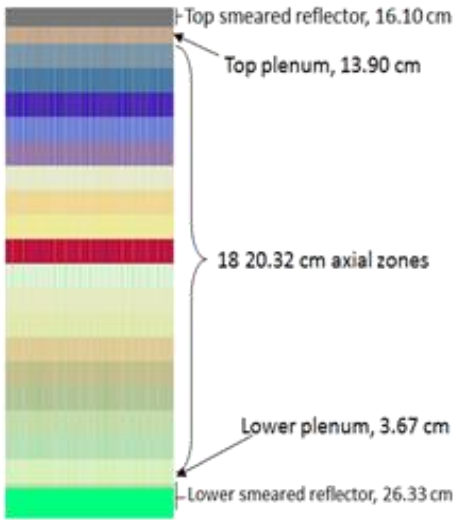
EGAMCT Benchmark Problems: Reactor Cases

Three Benchmark Cases:

R1 = 2D Core

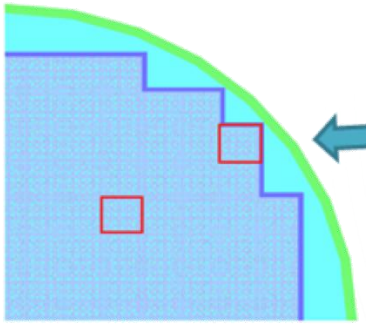
R2 = 3D Infinitely Reflected Assembly

R3 = 3D Core

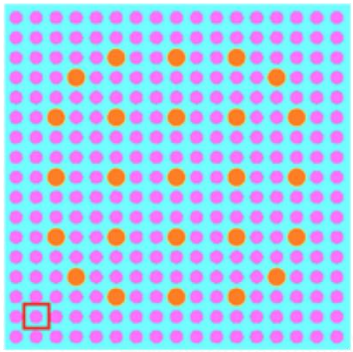


Assembly Axial Slices

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



Assembly Locations



Fuel Pin Location in each Assembly

[Perfetti and Rearden 2014]

EGAMCT Benchmark Problems: Shipping Cask Cases

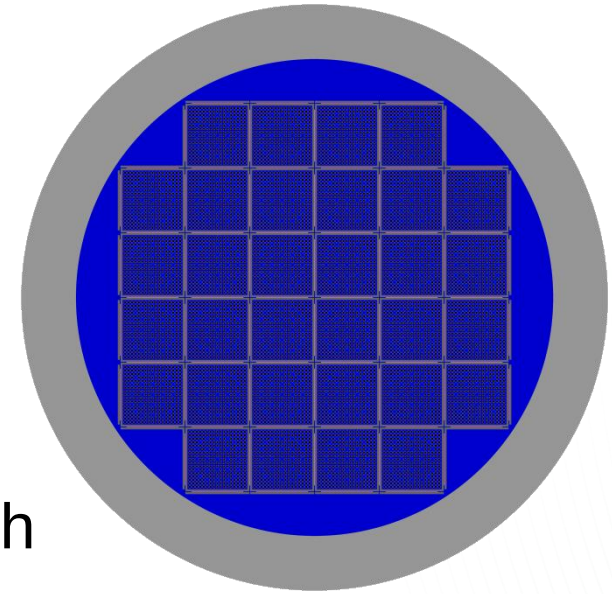
Three Benchmark Cases:

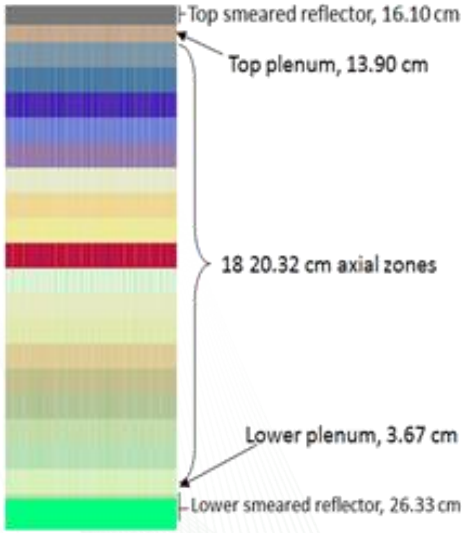
S1 = 2D Cask

S2 = 3D Infinitely Reflected Assembly

S3 = 3D Cask

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



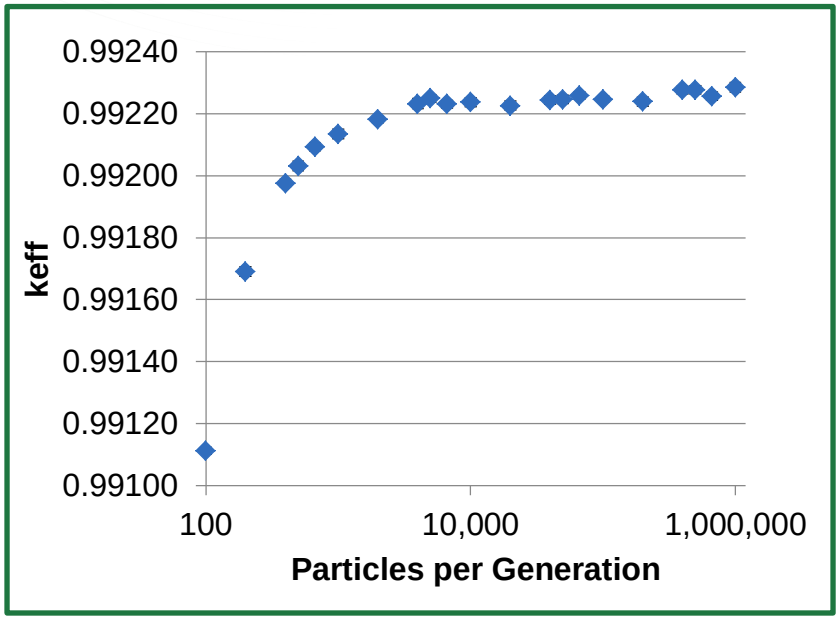


Assembly Axial Slices

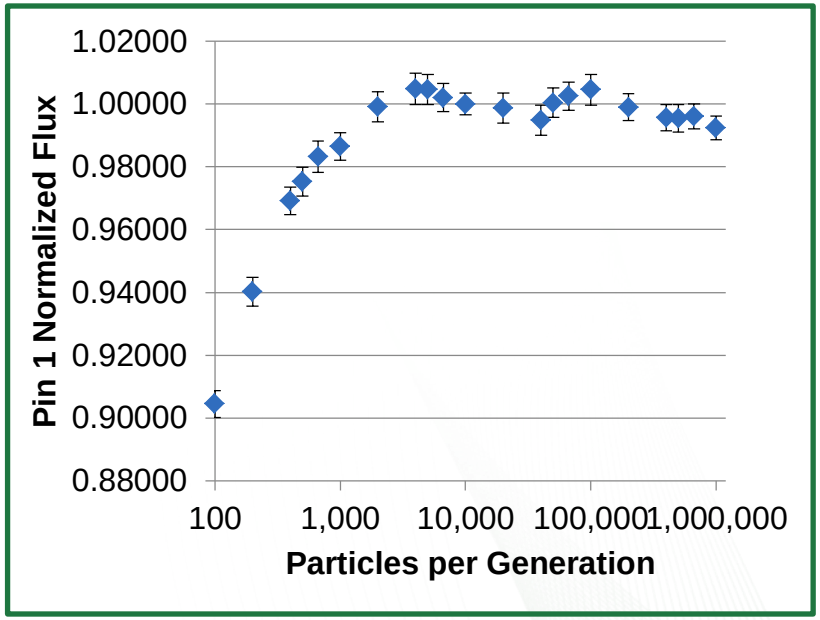
[Perfetti and Rearden 2014]

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.



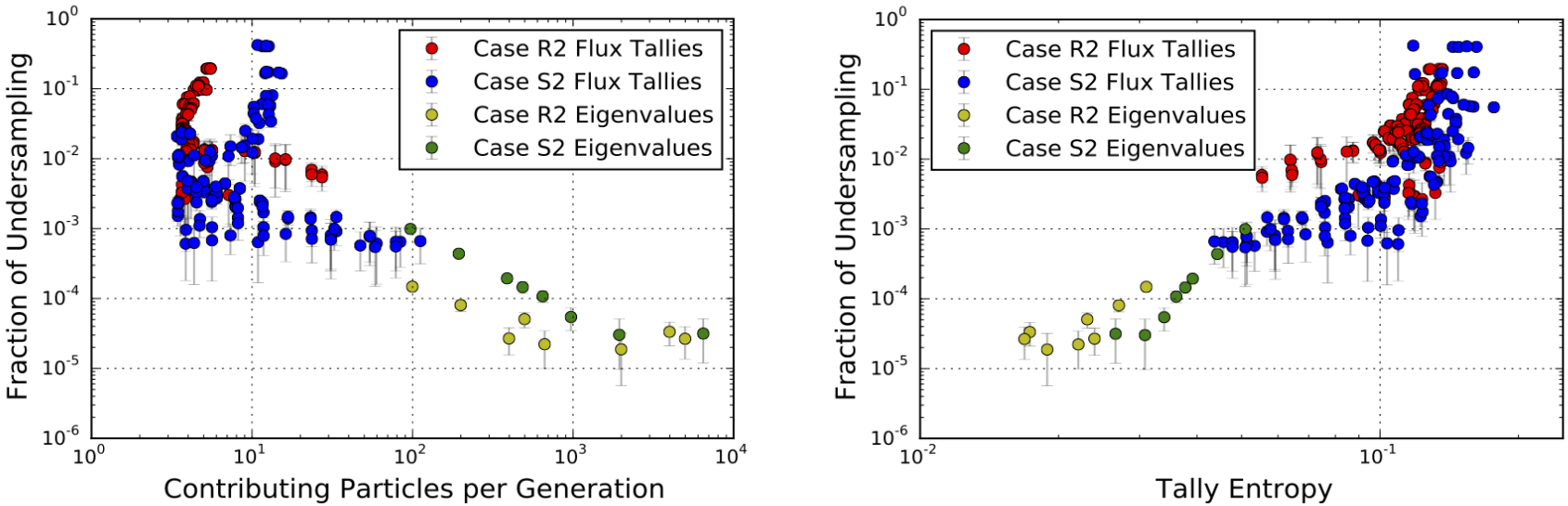
Undersampling in Case R1 eigenvalues [Perfetti and Rearden 2014]



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]

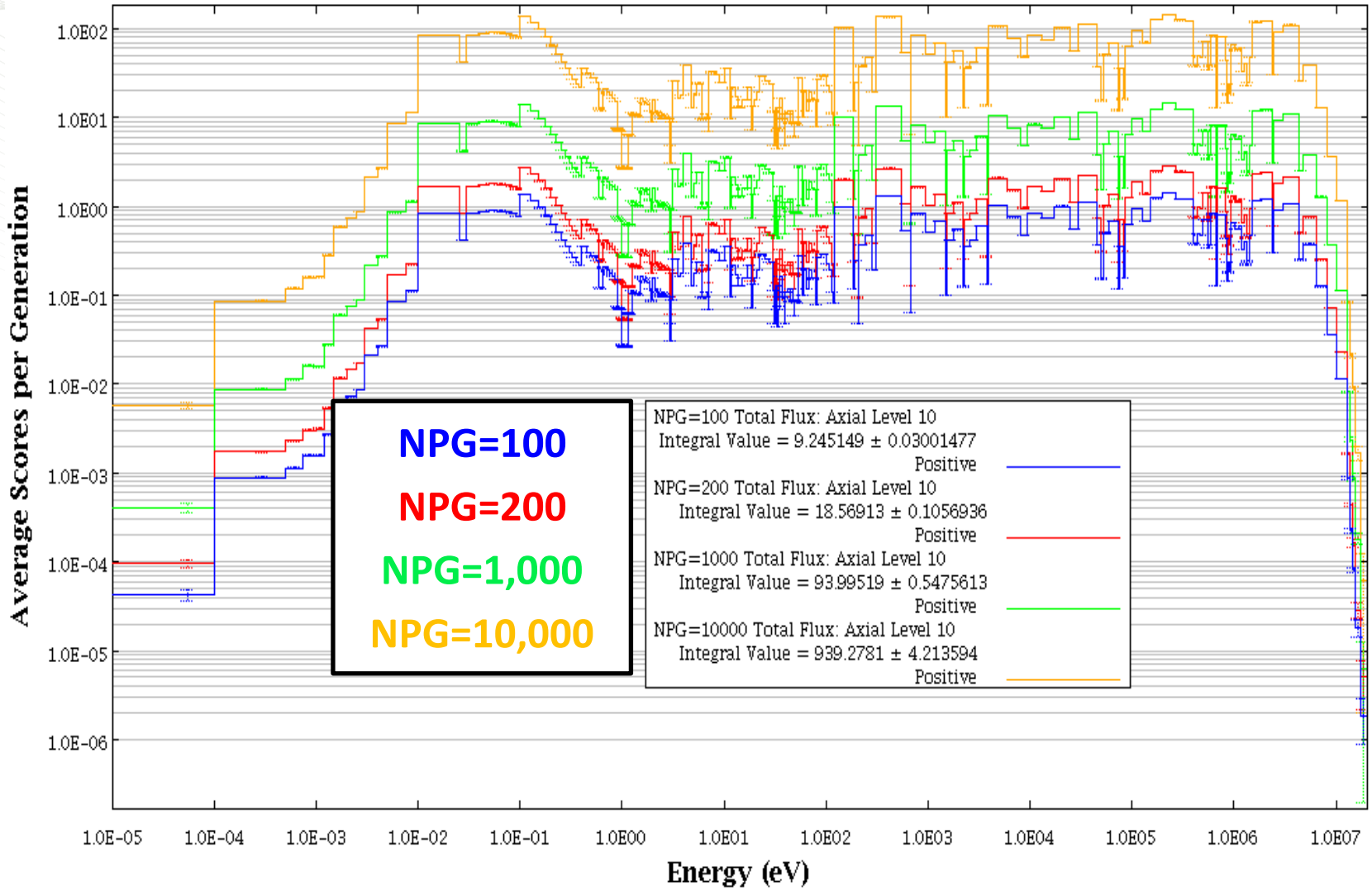
SCALE Undersampling Metrics

- Several undersampling metrics discussed in 2014 have been implemented within the CE TSUNAMI-3D framework of the SCALE 6.2 code package.
- These metrics can be enabled for a KENO model by running the TSUNAMI-3D-K5/6 sequence with the "cet=7" parameter.
- When enabled, undersampling metrics are calculated for:
  - $\mathbf{k_{eff}}$, the system's estimated eigenvalue,
  - $\boldsymbol{\phi}$**(E)**, the energy-dependent neutron flux in each material, and
  - **R(*nuc*,*mat*,*rxn*,E)**, the nuclide-dependent, energy-dependent reaction rates within each material.

SCALE 6.2 Undersampling Metrics

- A TSUNAMI undersampling metric calculation will produce the following undersampling metrics:
  - The overall tally score
  - The average number of tally scores per generation (SPGs)
  - Tally entropy
  - Heidelberger-Welch RHW
  - ~~Gekewe Z-Score~~
- These tallies are exported in SDF format for easy viewing and manipulation using Javapeño/Fulcrum

R2 Case: Number of Flux Tally Scores per Generation in the 10th Axial Level



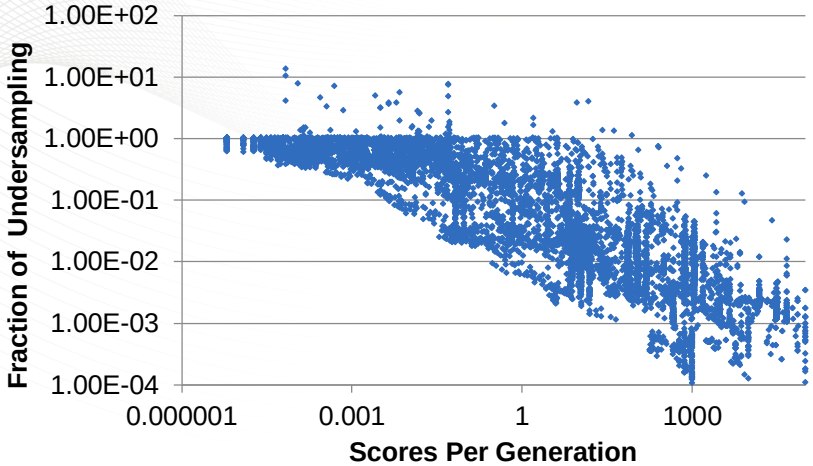
EGAMCT 2016 Collaboration Results

- In the 2015 EGAMCT collaboration these undersampling metrics were computed for all reaction rate, flux, and eigenvalue tallies for the S2 case and plotted against the undersampling bias (the *Fraction of Undersampling*).

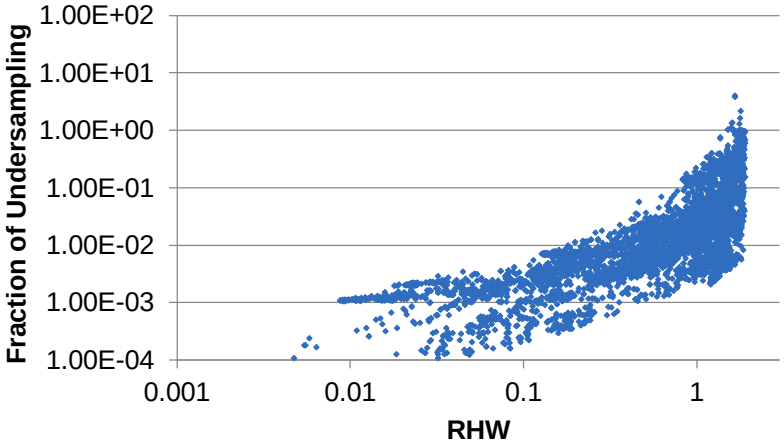
$$Fraction\ of\ Undersampling \equiv \frac{|Biased\ Score\ - Unbiased\ Score|}{Unbiased\ Score}$$

- These results contained a good deal of noise, making it difficult to draw substantial conclusions.

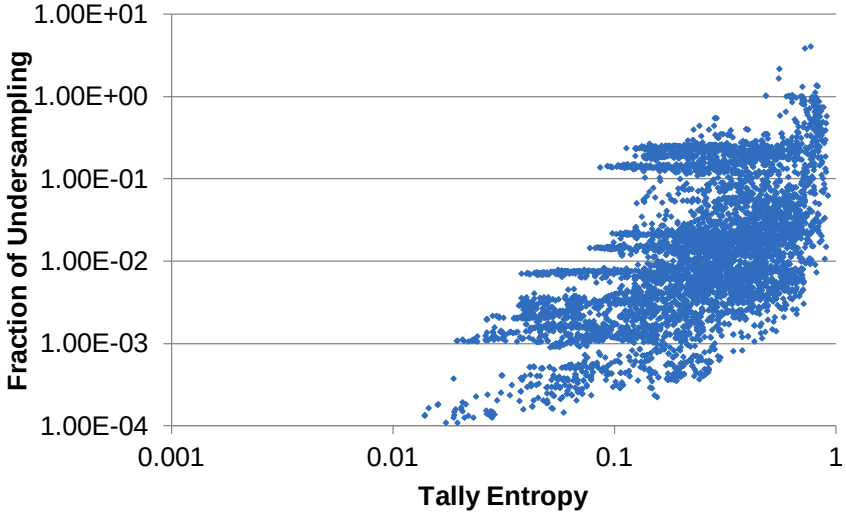
Background: S2 Results (2015)



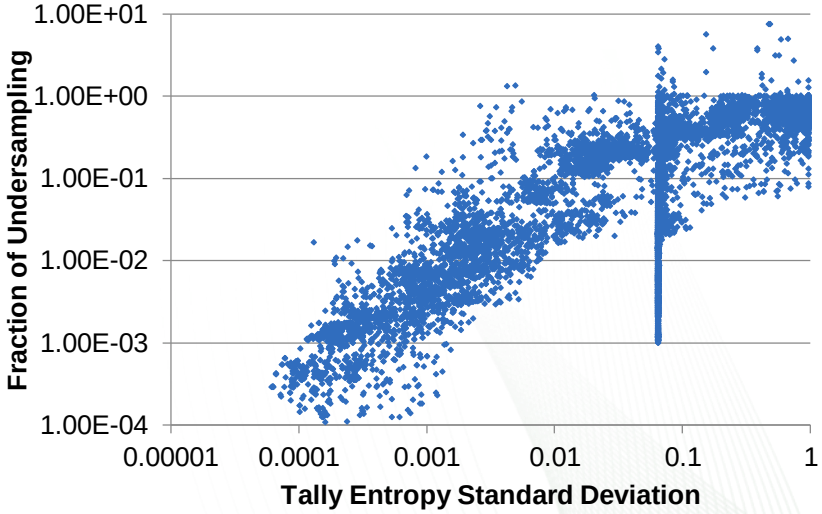
1) Scores Per Generation



2) Filtered RHW



3) Filtered Tally Entropy

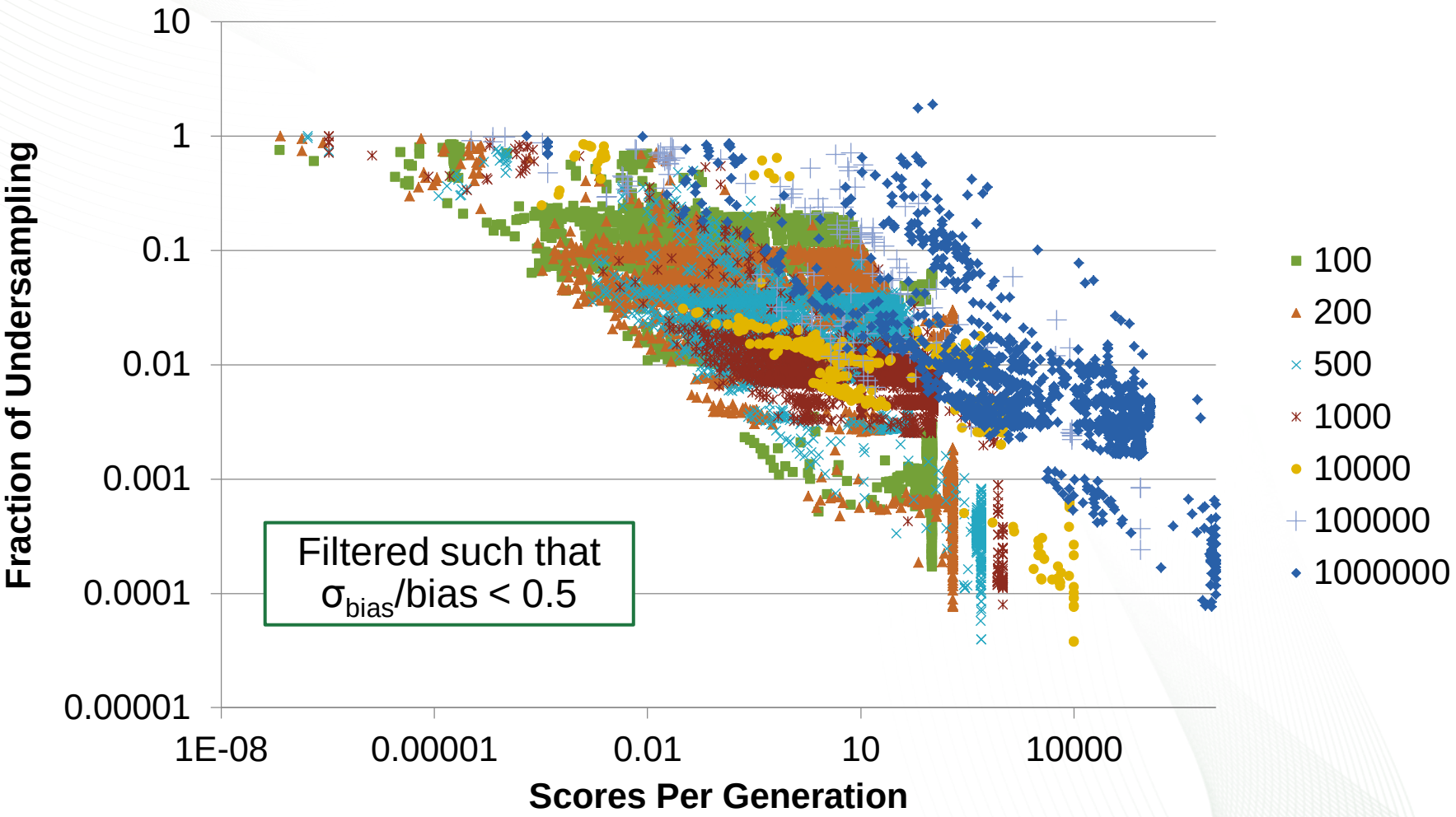


4) Tally Entropy St. Dev.

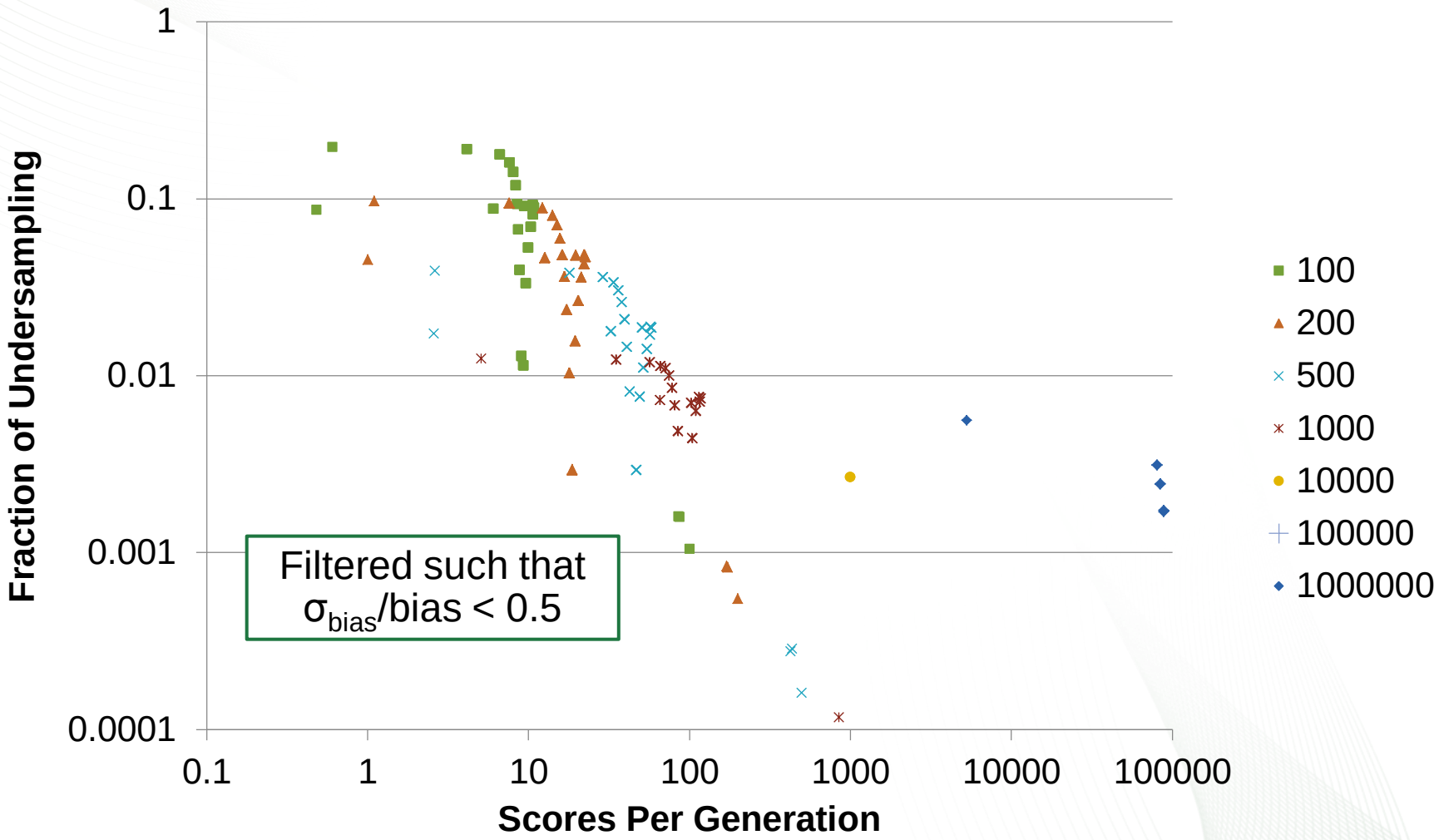
EGAMCT 2016 Collaboration Results

- In the past year, the CE TSUNAMI undersampling metrics were used to examine the undersampling bias in the R2 cases.
- These bias estimates were converged to a finer degree than those from 2015:
  - 20 times as many active histories were used in 2016 than in 2015.
- The reference results were obtained using 10 repeated simulations with 5,000,000 particles per generation (NPG) and 200 active generations.
- Repeated simulations were performed using NPG = 100, 200, 500, 1,000, 10,000, 100,000, and 1,000,000.

Average Number of Tally Scores per Generation (SPG)



Average Number of Tally Scores per Generation (SPG): Flux Tallies Only



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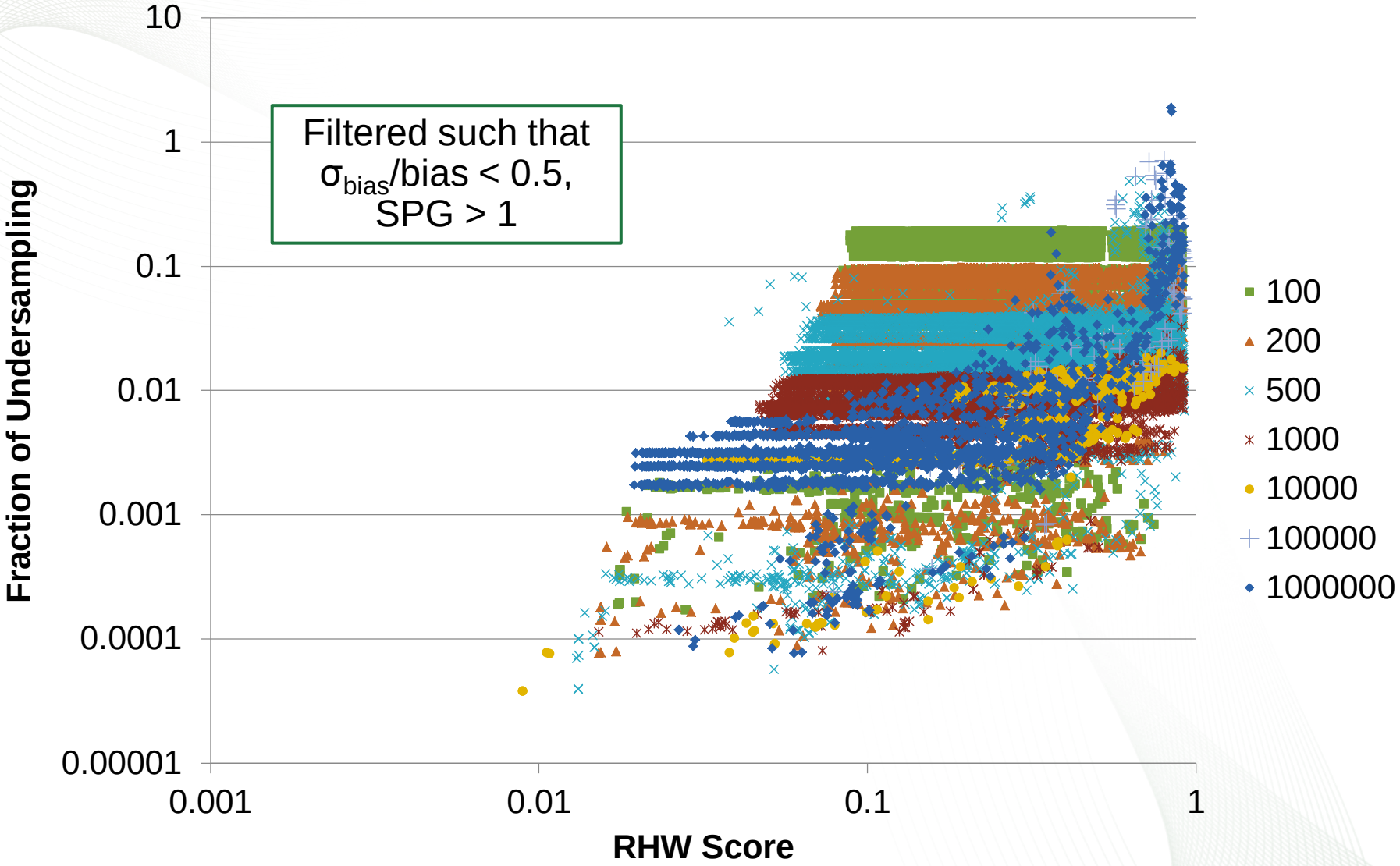
Heidelberger–Welch RHW

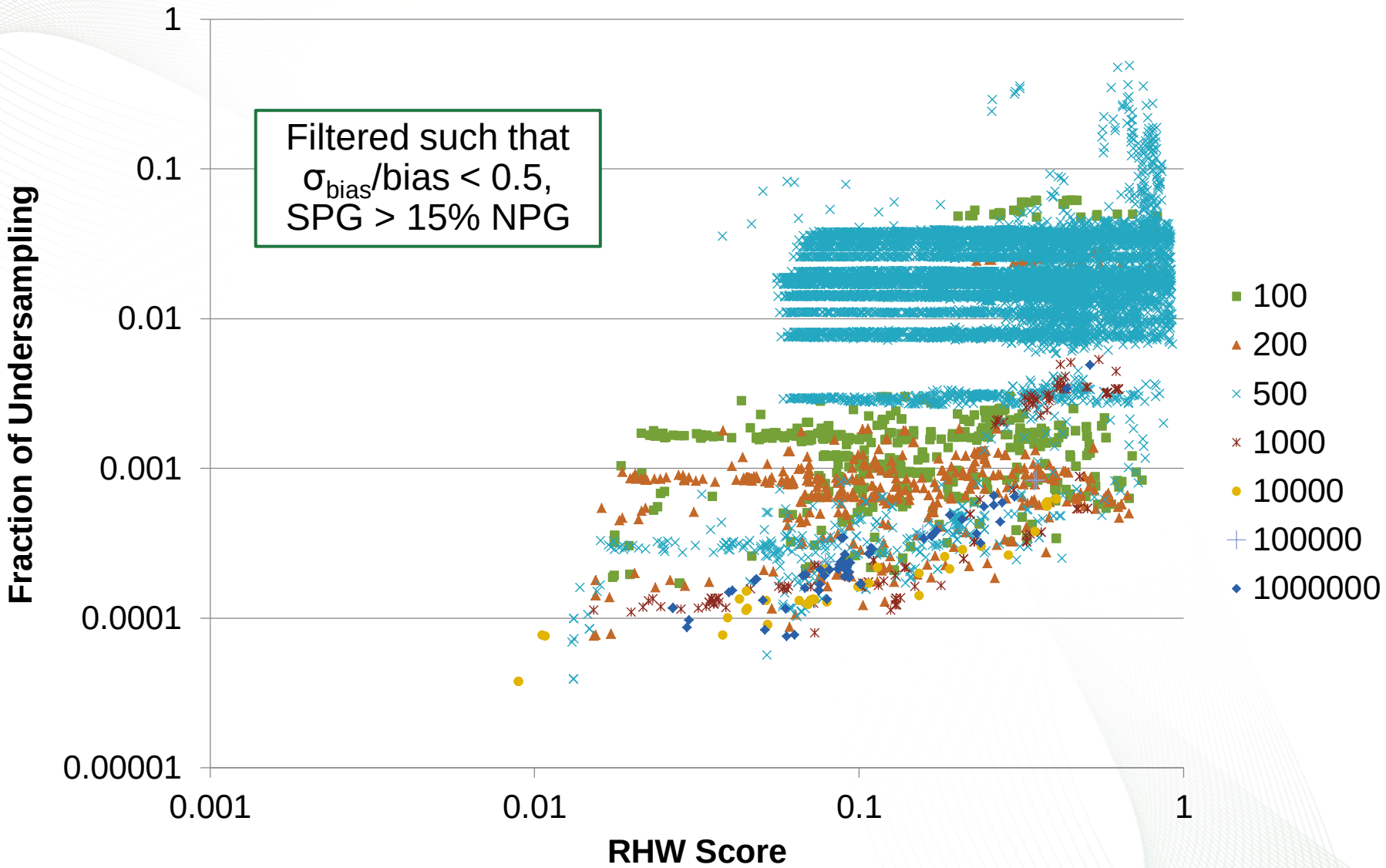
The Heidelberger–Welch Relative Half-Width (RHW) test assesses convergence by determining if the samples within a Markov chain vary significantly outside the confidence interval (α) of that chain.

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

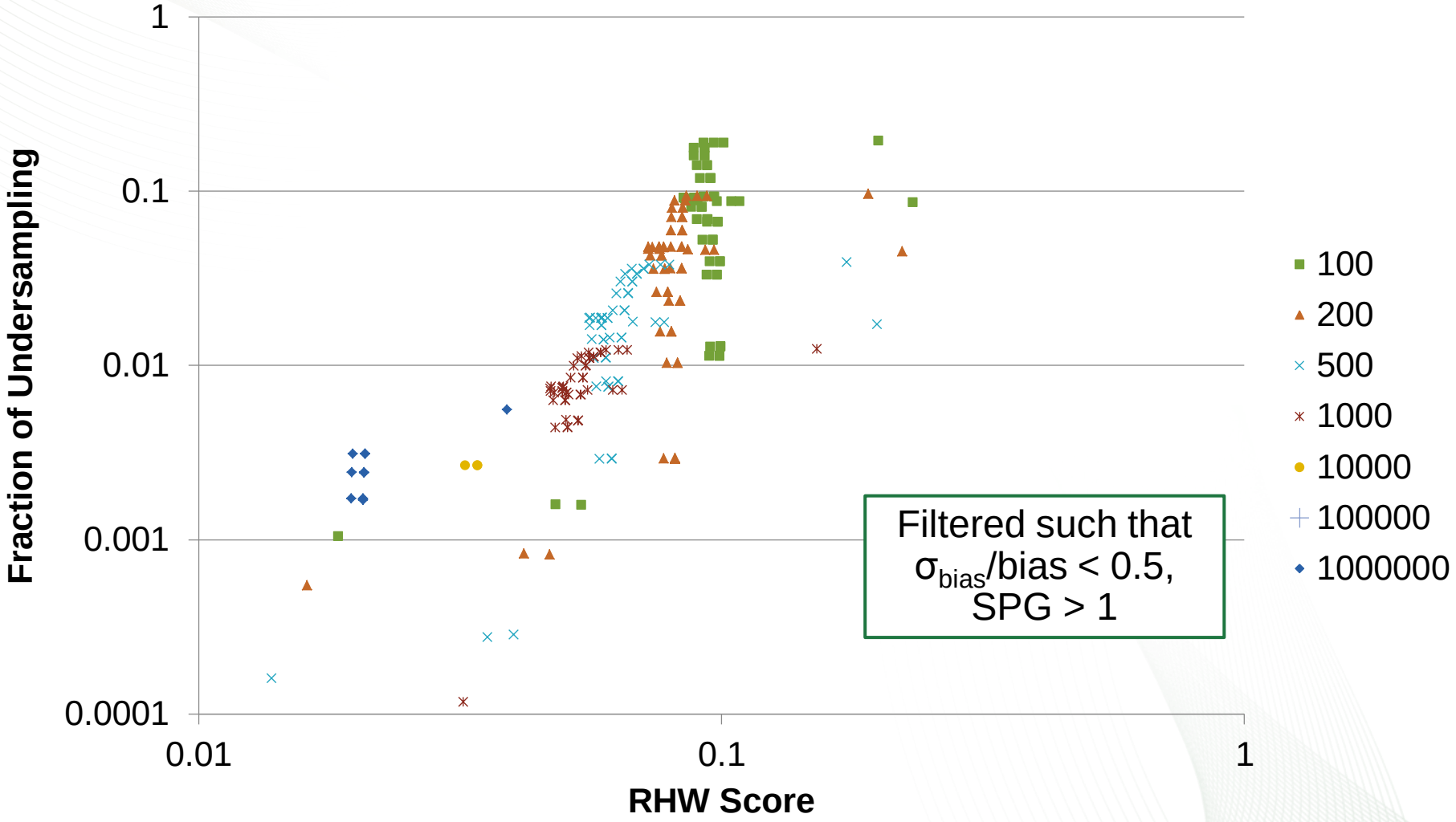
Heidelberger–Welch RHW



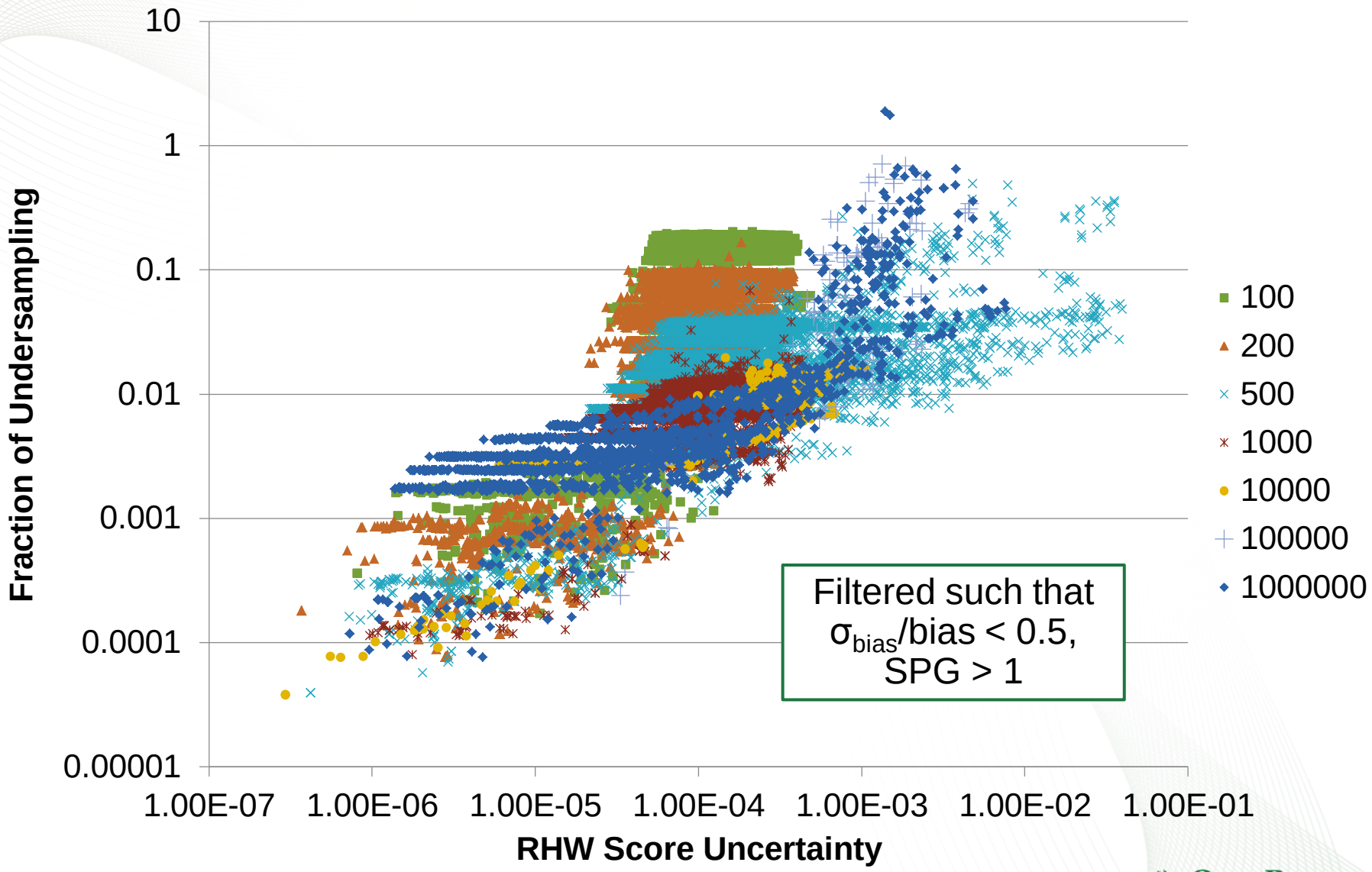
Heidelberger–Welch RHW



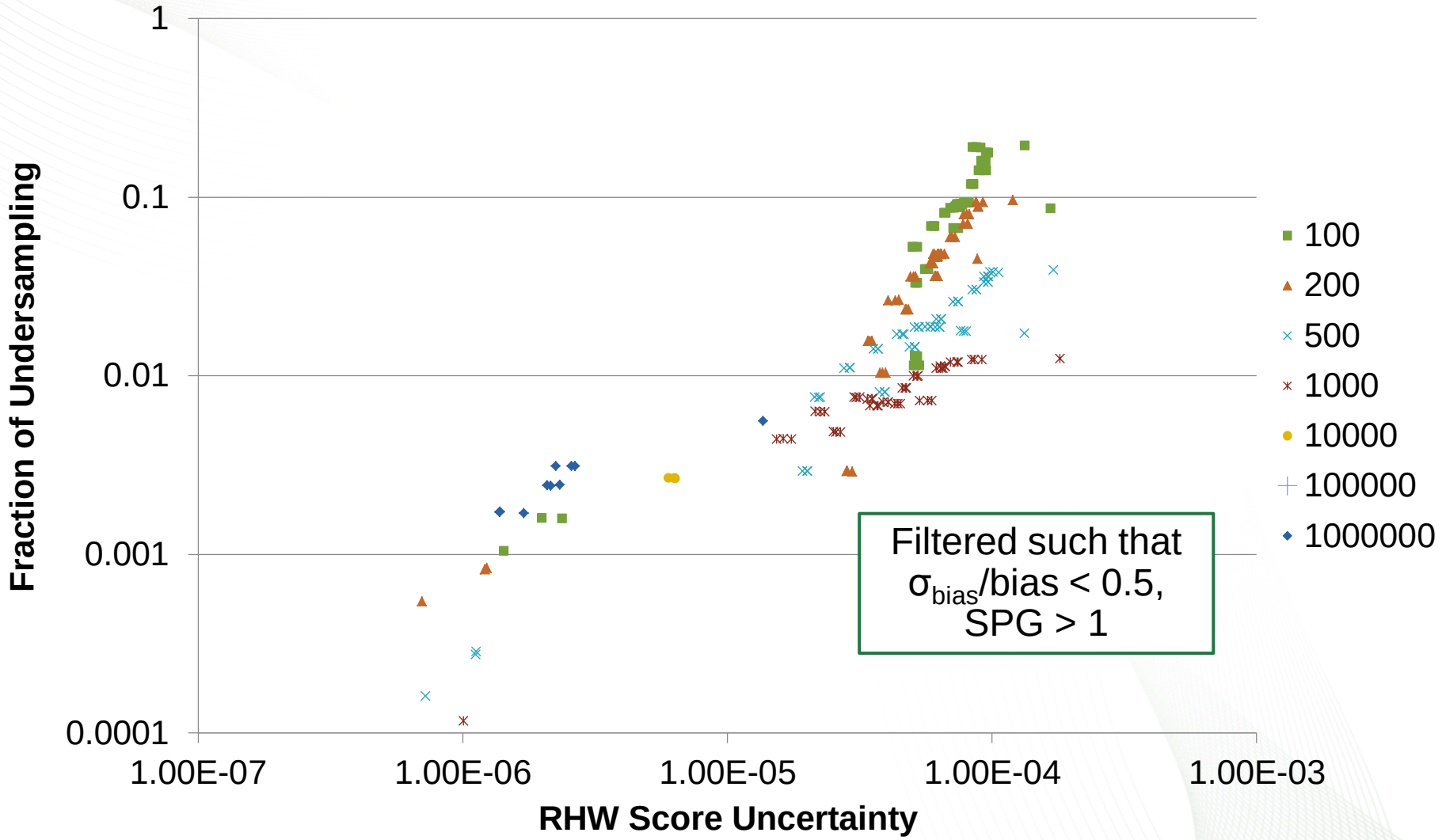
Heidelberger–Welch RHW: Flux Tallies Only



RHW Score Uncertainty:



RHW Score Uncertainty: Flux Tallies Only



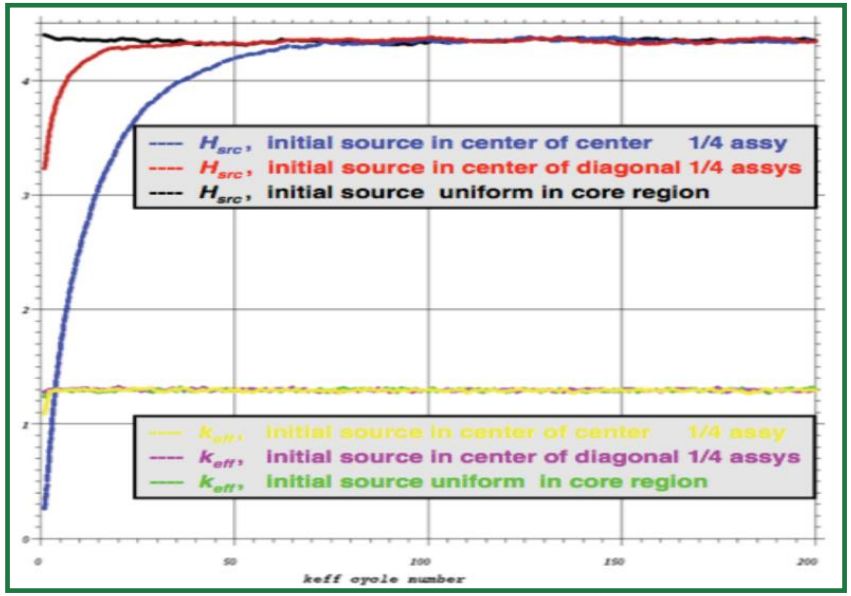
Tally Entropy: A New Diagnostic

- Shannon entropy is a concept from information theory that measures the amount of information contained in messages in a data stream.

$$H = -\sum_{n}^{N} p_n \ln(p_n)$$

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

- Brown and Ueki have applied 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. 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.

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

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

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.

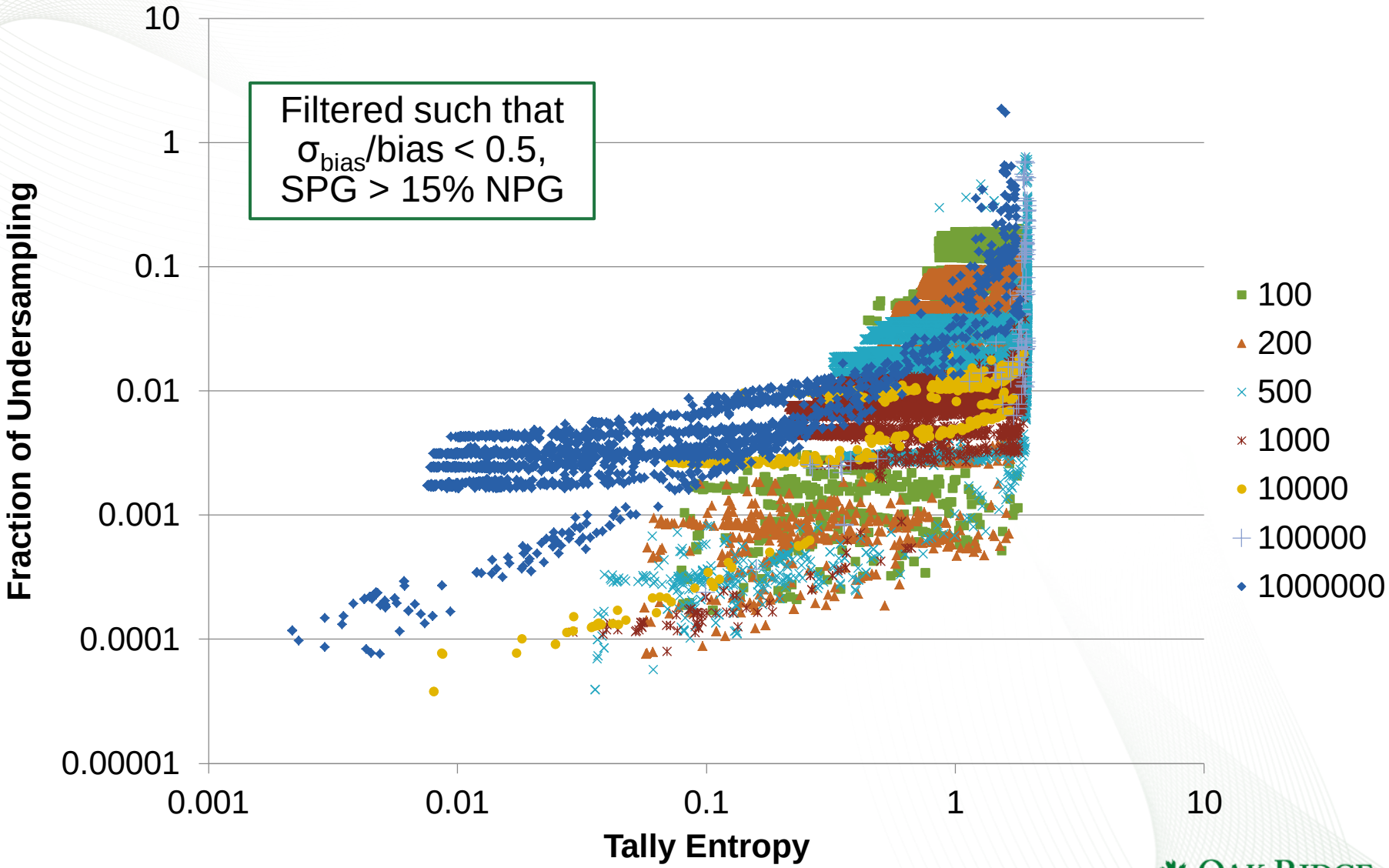
$$H = -\sum_{n}^{N} p_n \ln(p_n)$$

These are ideal conditions for preventing undersampling.

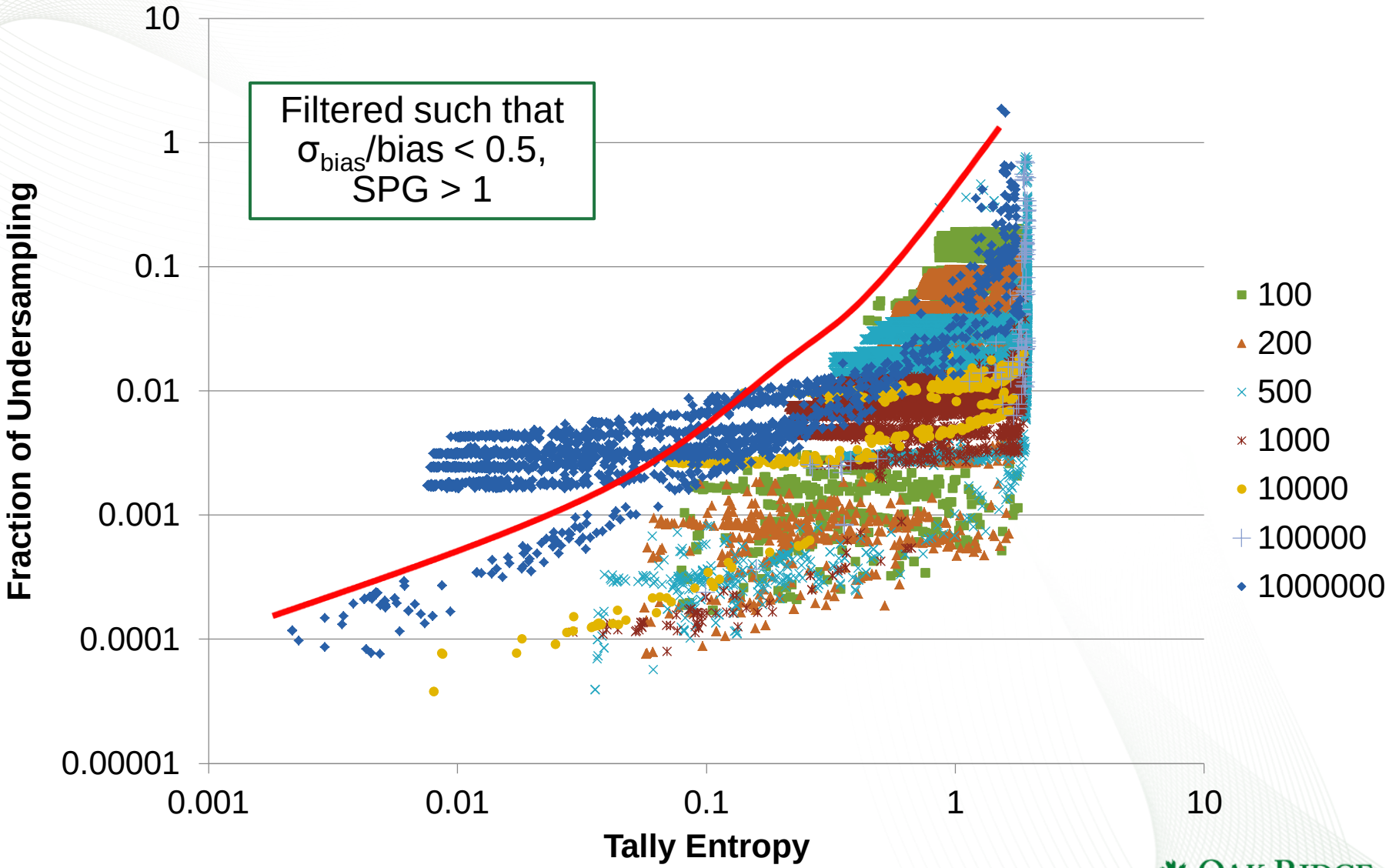
- A new test statistic was developed by examining the fractional difference between the entropy of a tally, H_i, and its limit of $\ln(N_i)$:

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

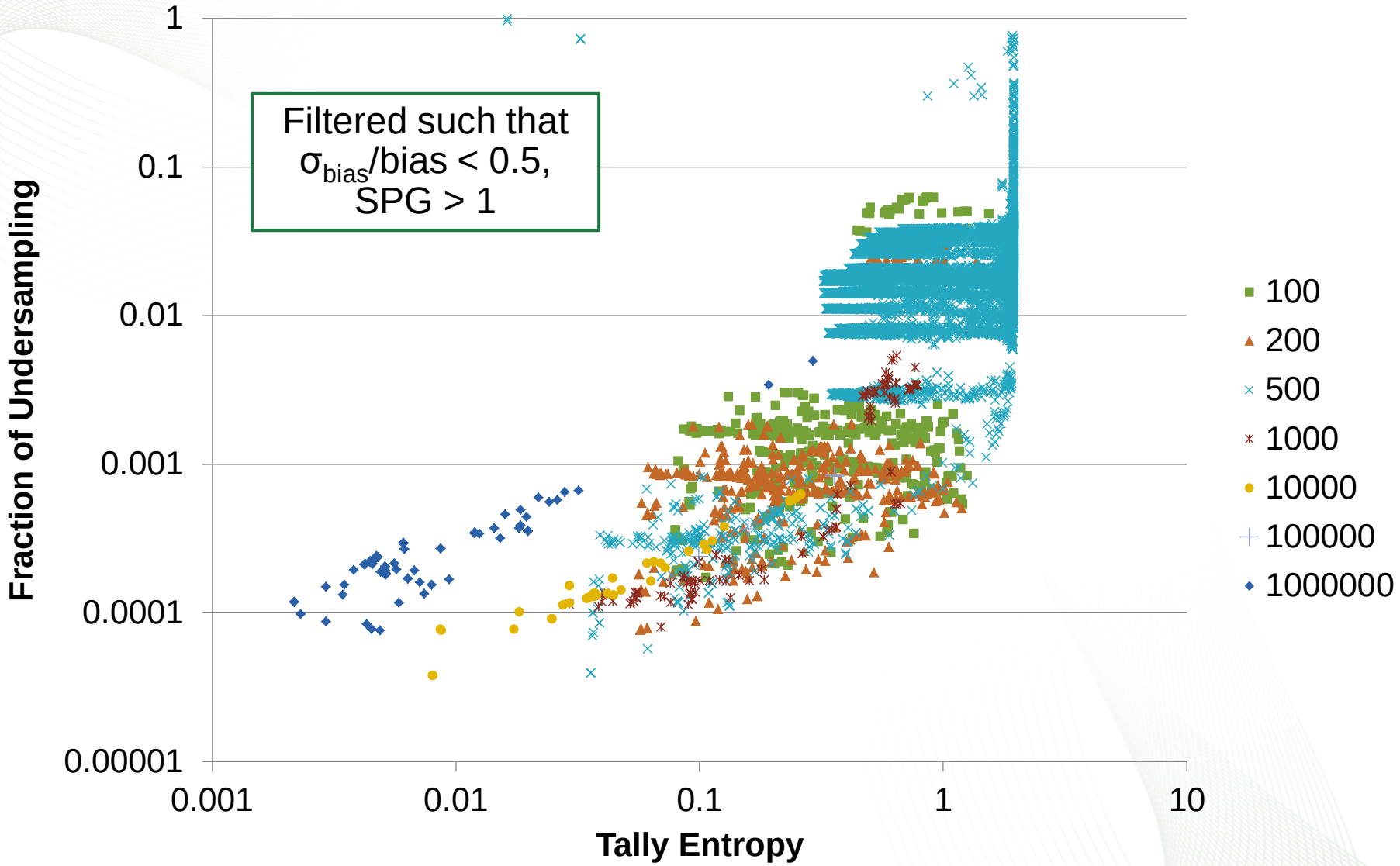
Tally Entropy



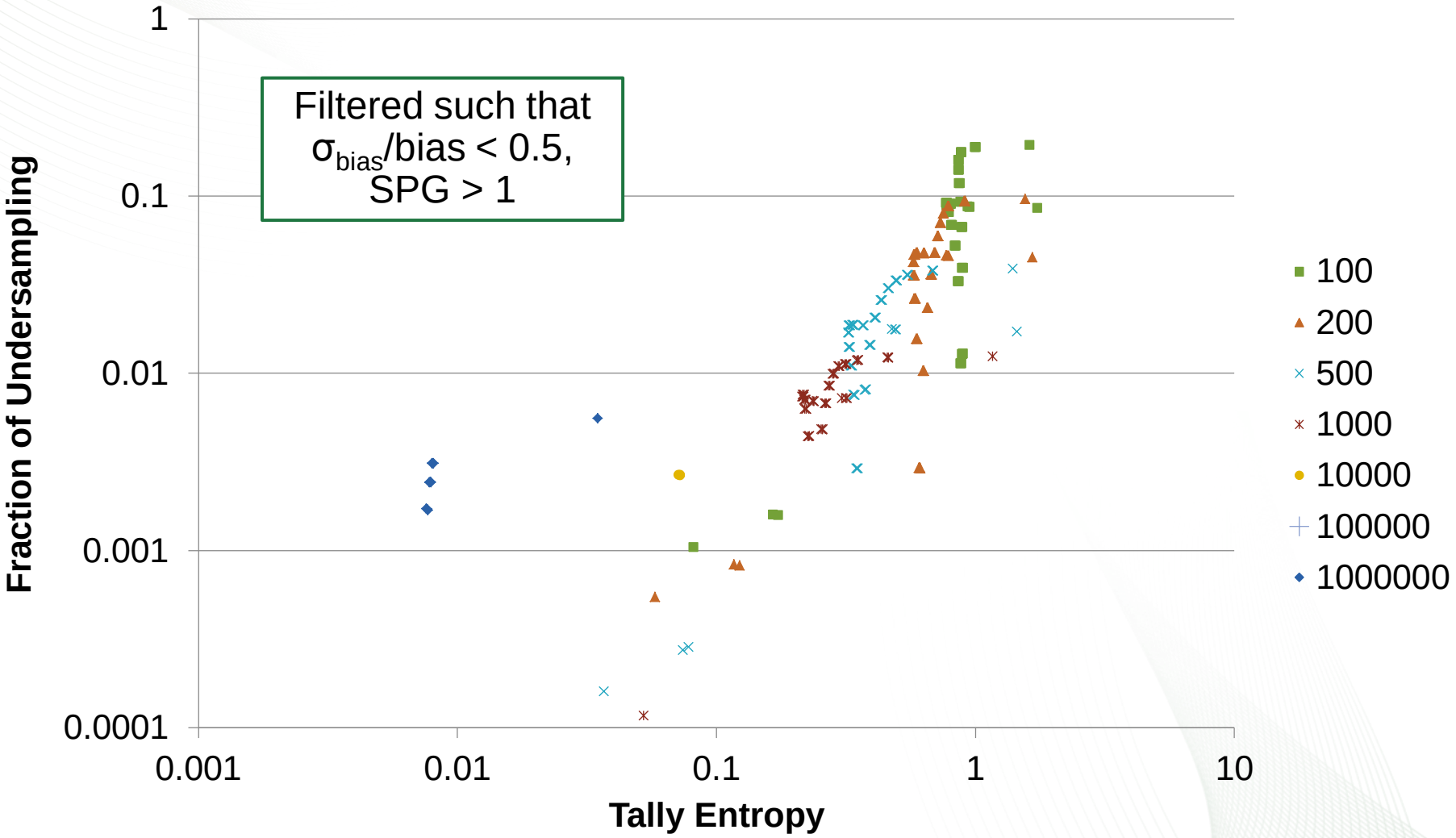
Tally Entropy



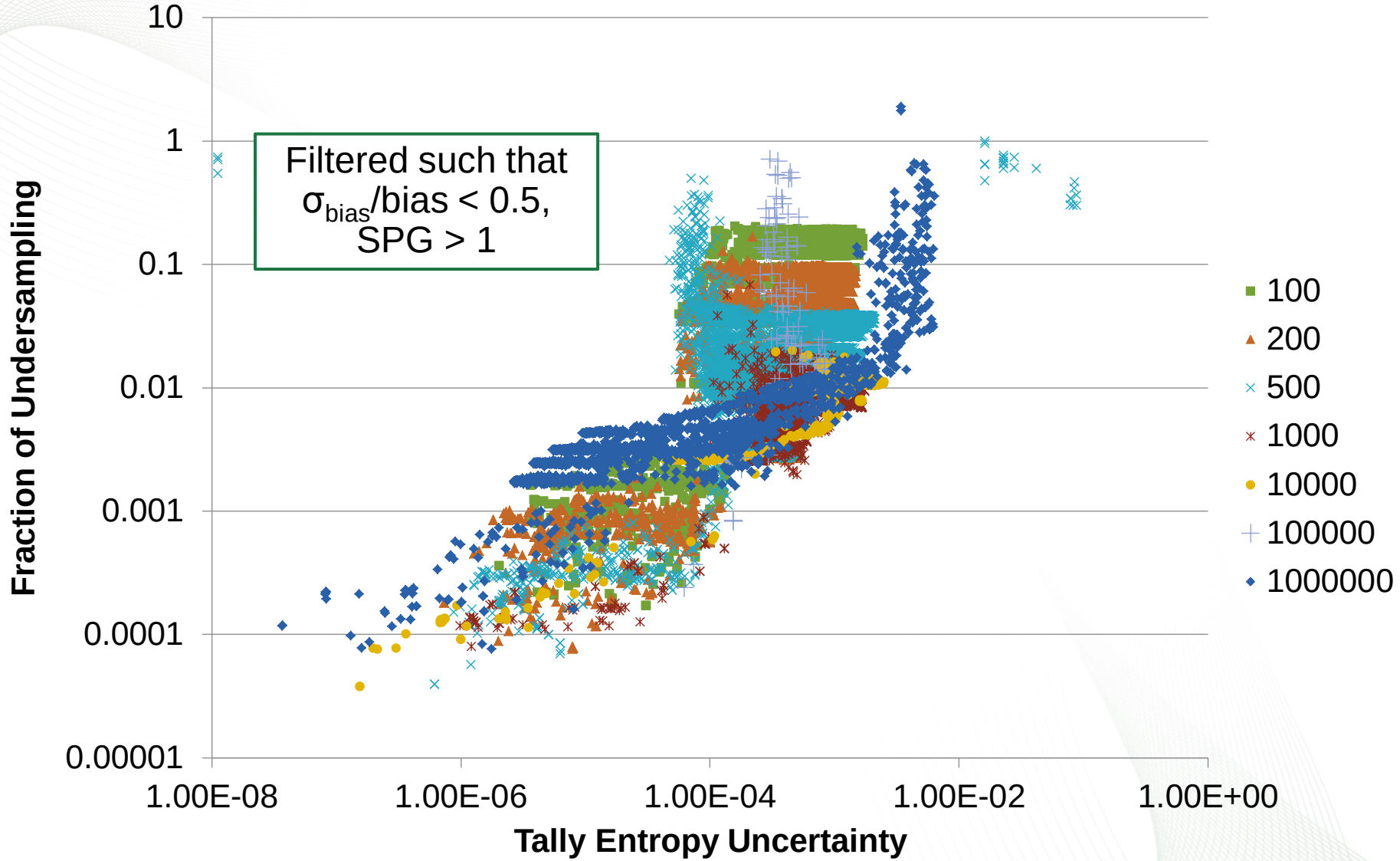
Tally Entropy



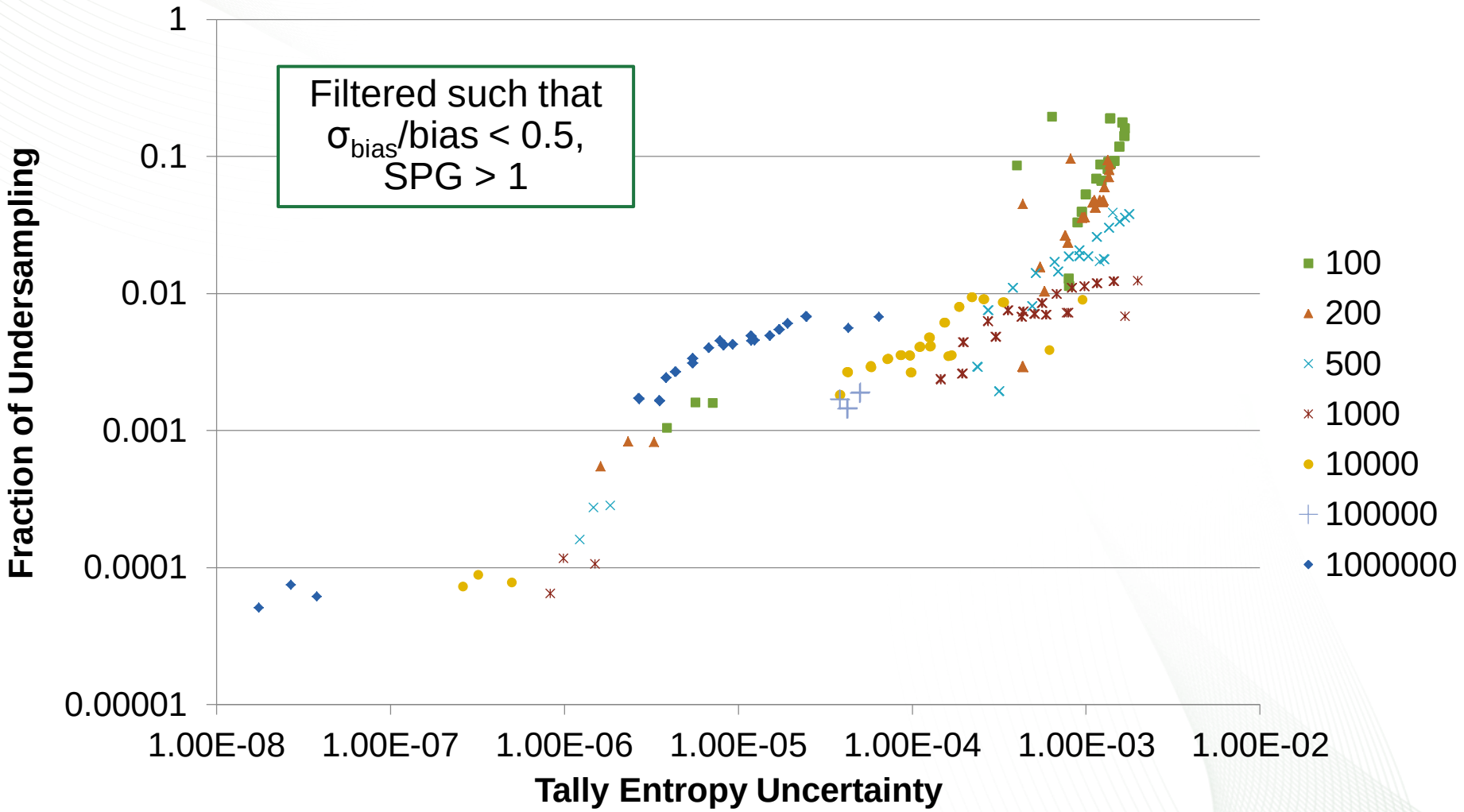
Tally Entropy: Flux Tallies Only



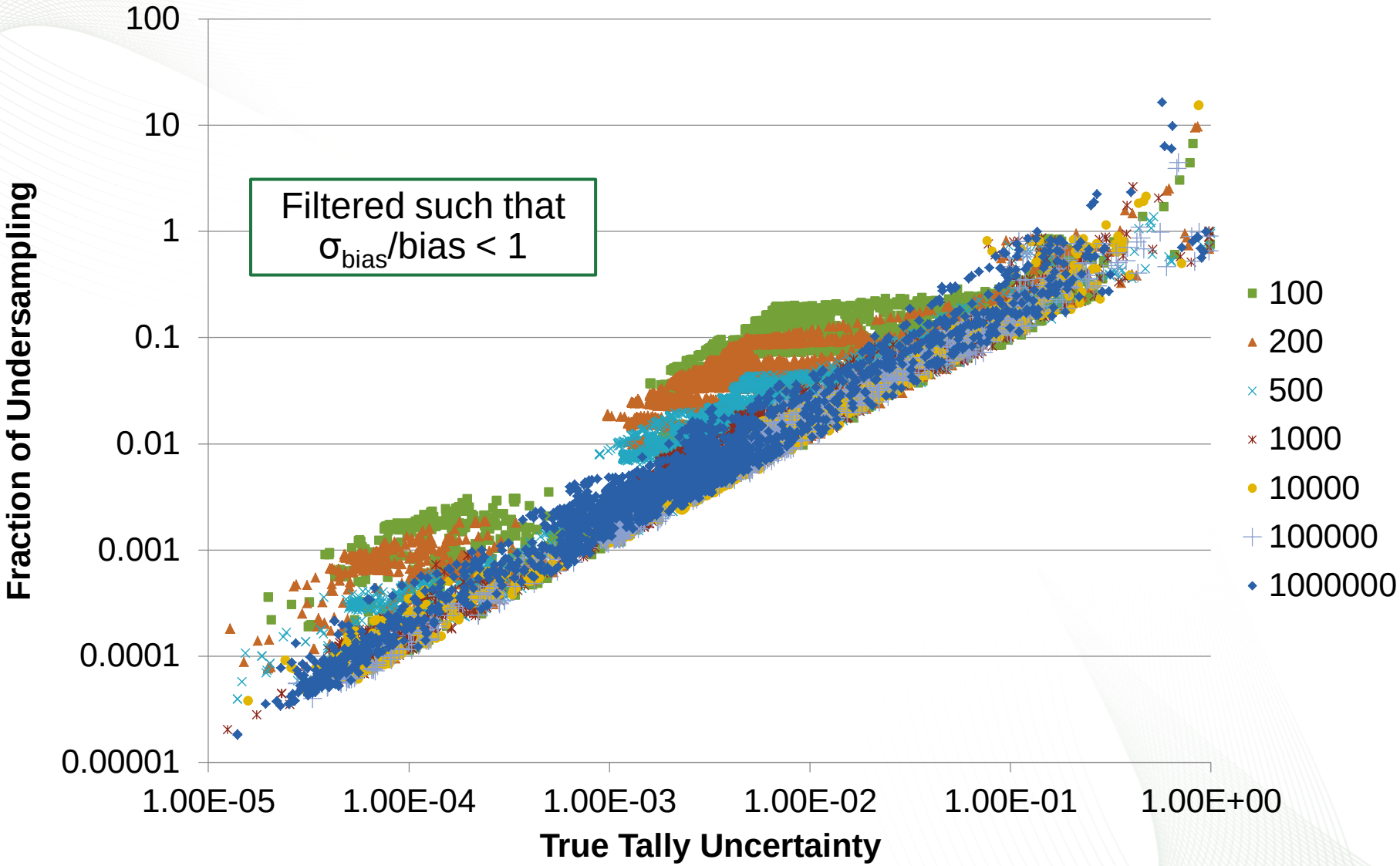
Tally Entropy Uncertainty



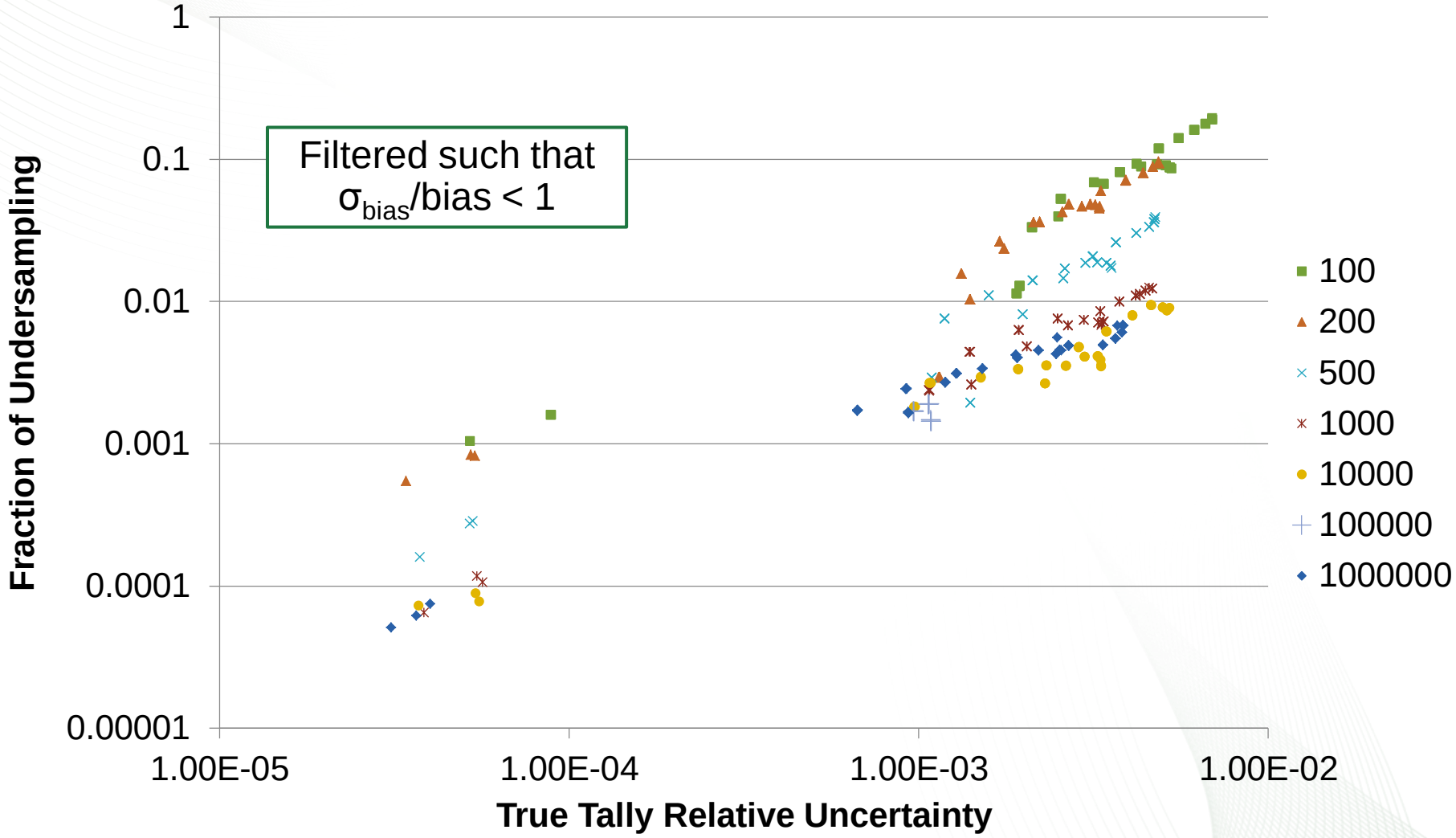
Tally Entropy Uncertainty: Flux Tallies Only



True Tally Uncertainty:



True Tally Uncertainty: Flux Tallies Only



Conclusions

- Although a significant amount of noise still exists in the bias information, the undersampling metrics were not found to be especially effective at predicting the magnitude of the undersampling biases.
- Of the metrics examined, the RHW and Tally Entropy metrics were somewhat effective at predicting the undersampling biases, especially when combined with SPG filtering.
- The true tally uncertainty also seemed somewhat effective at predicting the undersampling biases.
- Future EGAMCT collaborations could benefit from developing additional metrics for detecting undersampling biases.

Questions???

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