Ensuring the Fidelity of Data Assimilation Methodology Bias Estimates

...aka...

Tsurfer Tstudies

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Challenges for Data Assimilation

1. Are any of the experiments outliers or erroneous?

2. Can the experiments be treated as independent data points?
   Are any of the experiments correlated?

3. Is the solution under-constrained?
   Are we using enough experiments?

4. Is the covariance data accurate, or at least "good enough" ?

5. How do we get a 95/95 confidence interval from these results?

Challenges for Data Assimilation

1. Are any of the experiments outliers or erroneous?

➔ **Delta Chi-squared filtering used to detect inconsistent experiments.**

$$\Delta\chi_i^2 = \chi_{All\ Exp.}^2 - \chi_{Omit\ Exp.\ i}^2$$

Challenges for Data Assimilation

2. Can the experiments be treated as independent data points?
   Are any of the experiments correlated?

➔ **Only uncorrelated experiments were used in this study. SDFs were generated for a total of 56 experiments taken from:**

1. The ORNL Valid Library
2. ICSBEP Sample Inputs
3. The BFS Experiments [1]

[1] E. Ivanov, "Approach and issues of covariance matrix establishment for systems with variable spectra," presented at GRS, Garching, Germany (2016).

Challenges for Data Assimilation

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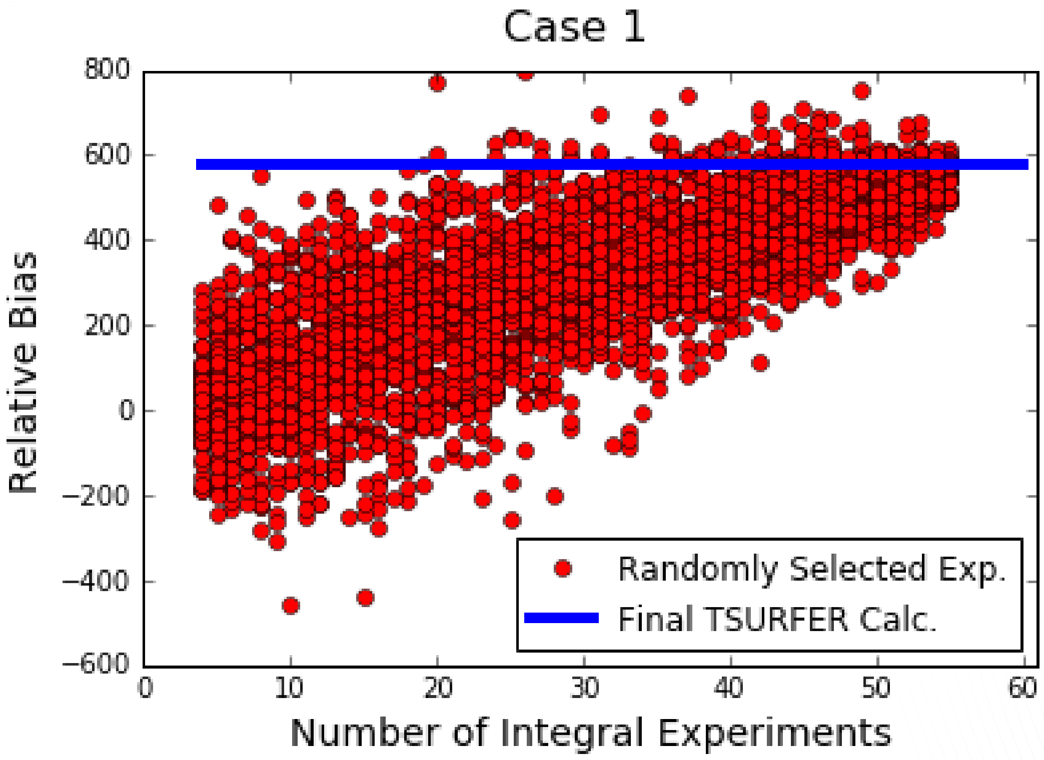
➔ **Convergence was assessed by re-simulating the TSURFER calculation while randomly omitting experiments.**

- The number of randomly omitted experiments was varied for the TSURFER simulation.
  - Convergence should be apparent as the number of randomly omitted experiments approaches zero.
  - 60 random realizations were simulated for each number of omitted experiments.

Results – 56-group Covariance, 56 Exp.



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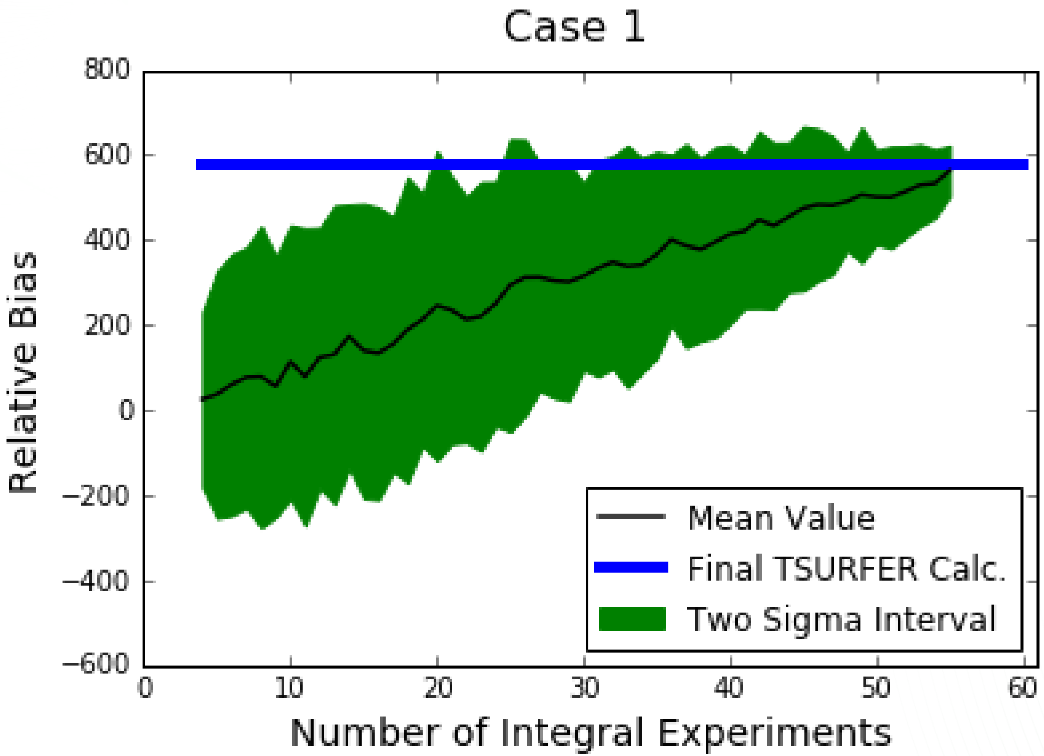

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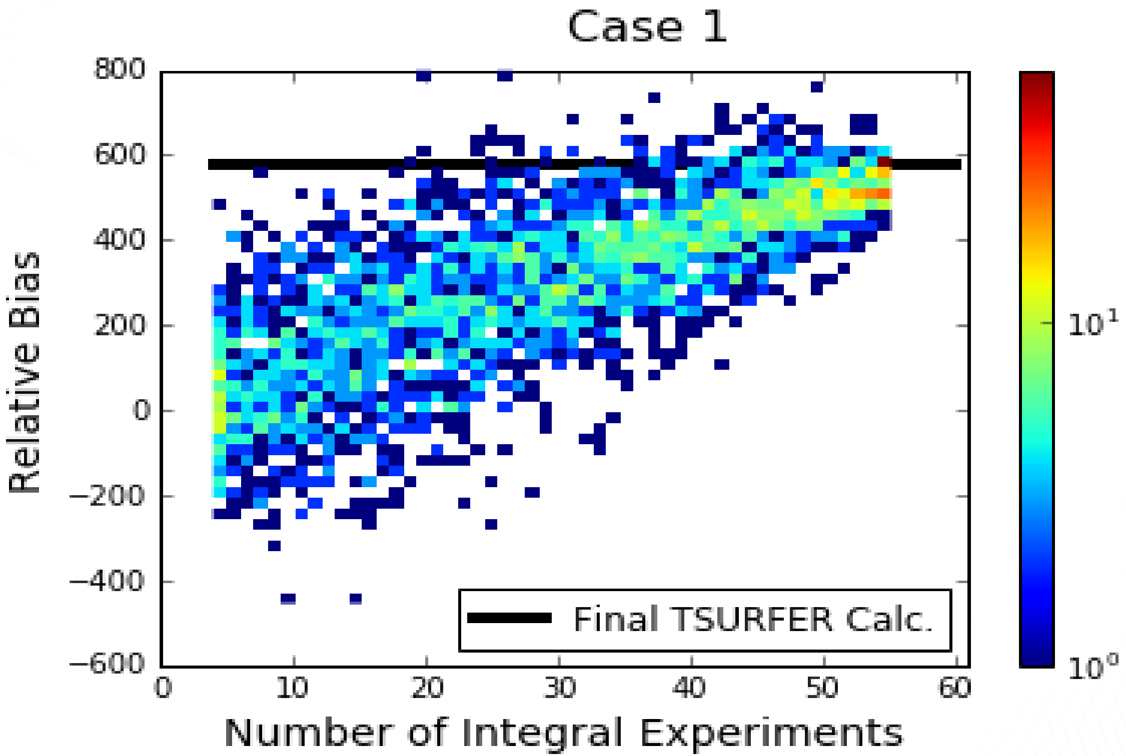
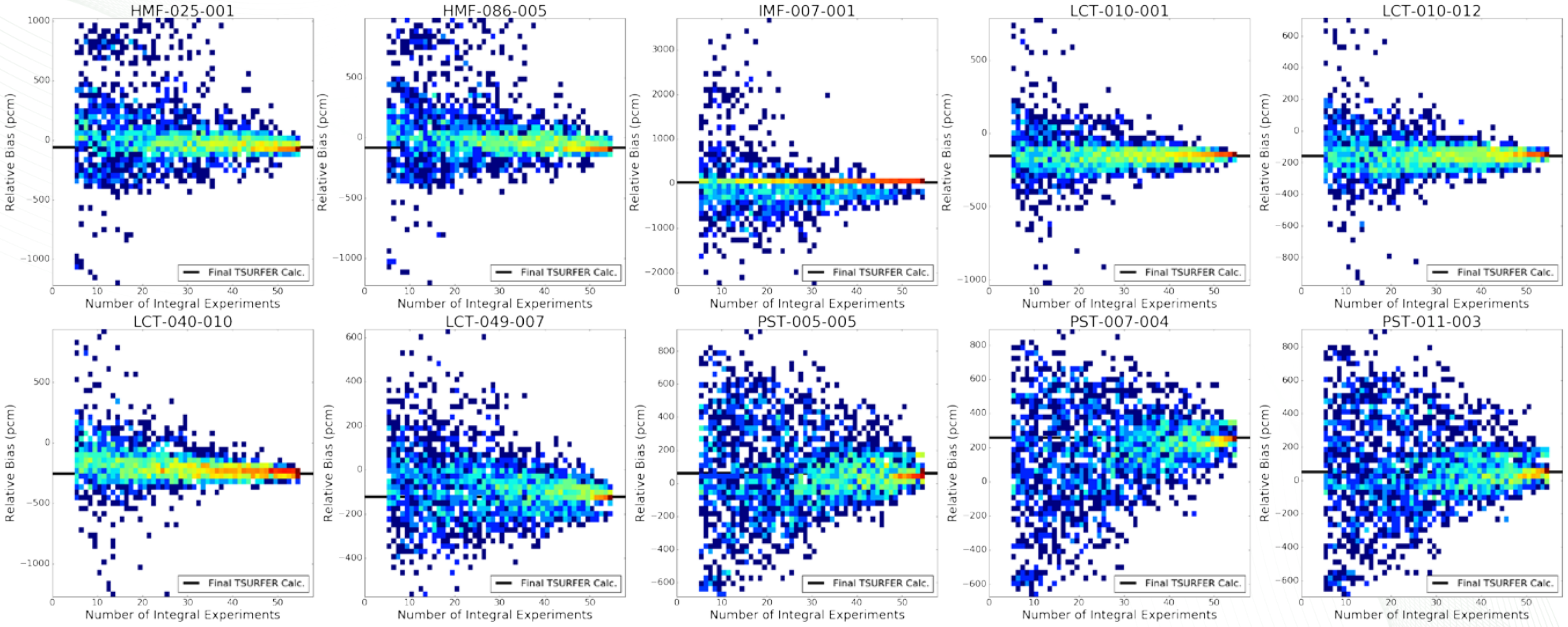


Known Bias Cases – 56-group Covariance, 56 Exp.



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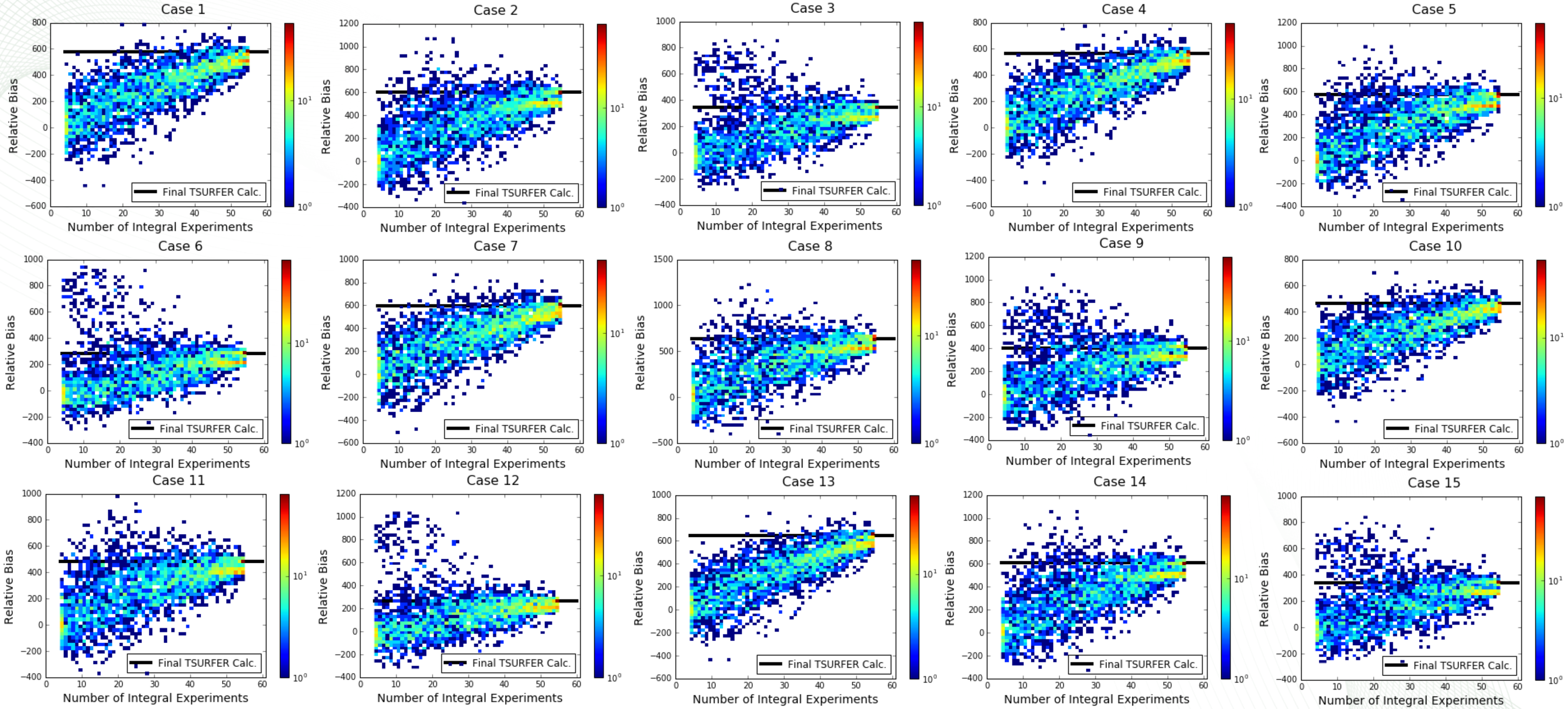
Unknown Bias Cases – 56-group Covariance, 56 Exp.



Challenges for Data Assimilation

3. Is the TSURFER solution under-constrained?

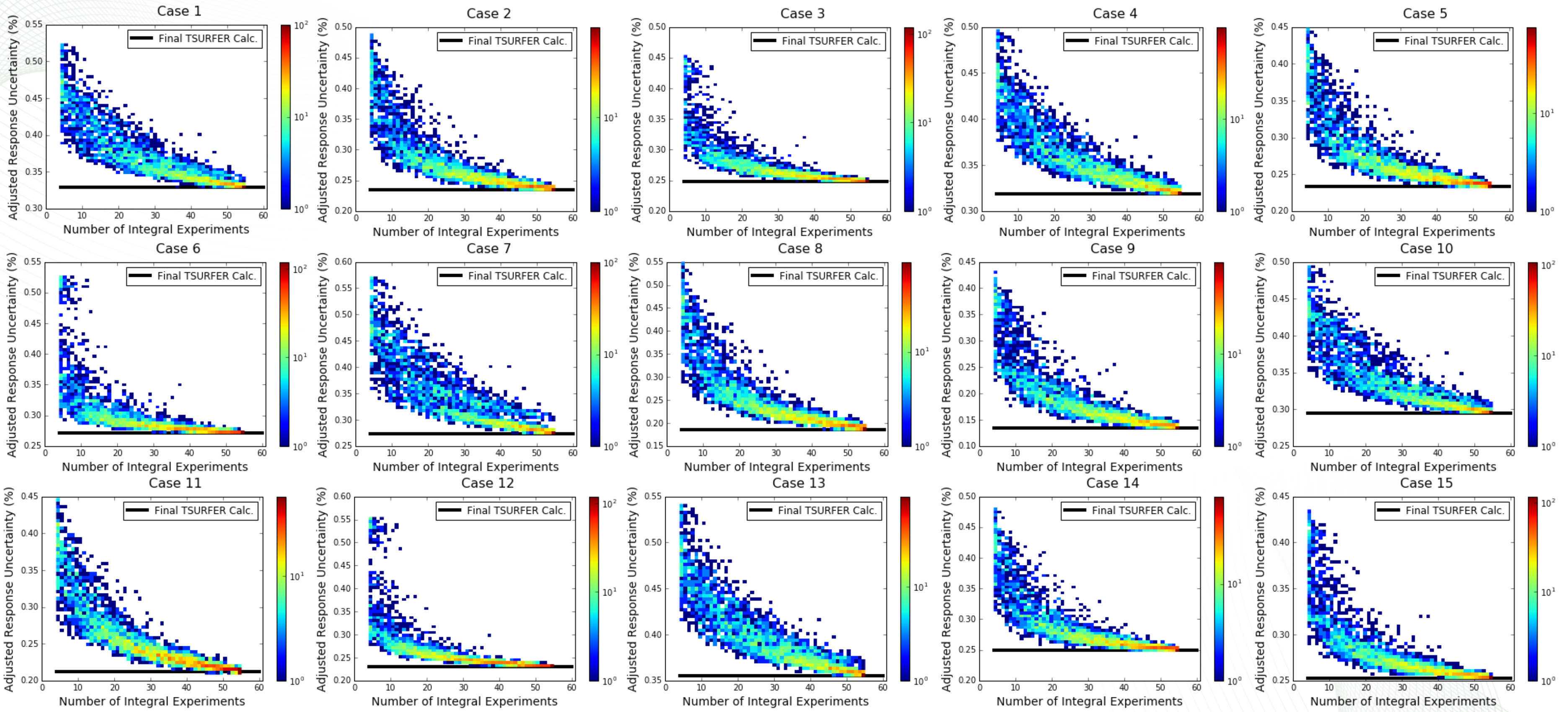
   Are we using enough experiments?

   How else can we assess convergence?

➔ **Examine the convergence of the data-induced uncertainty in the adjusted response.**

➔ **Add more experiments.**

Response Uncertainty Convergence – 56-grp., 56 Exp.



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Challenges for Data Assimilation

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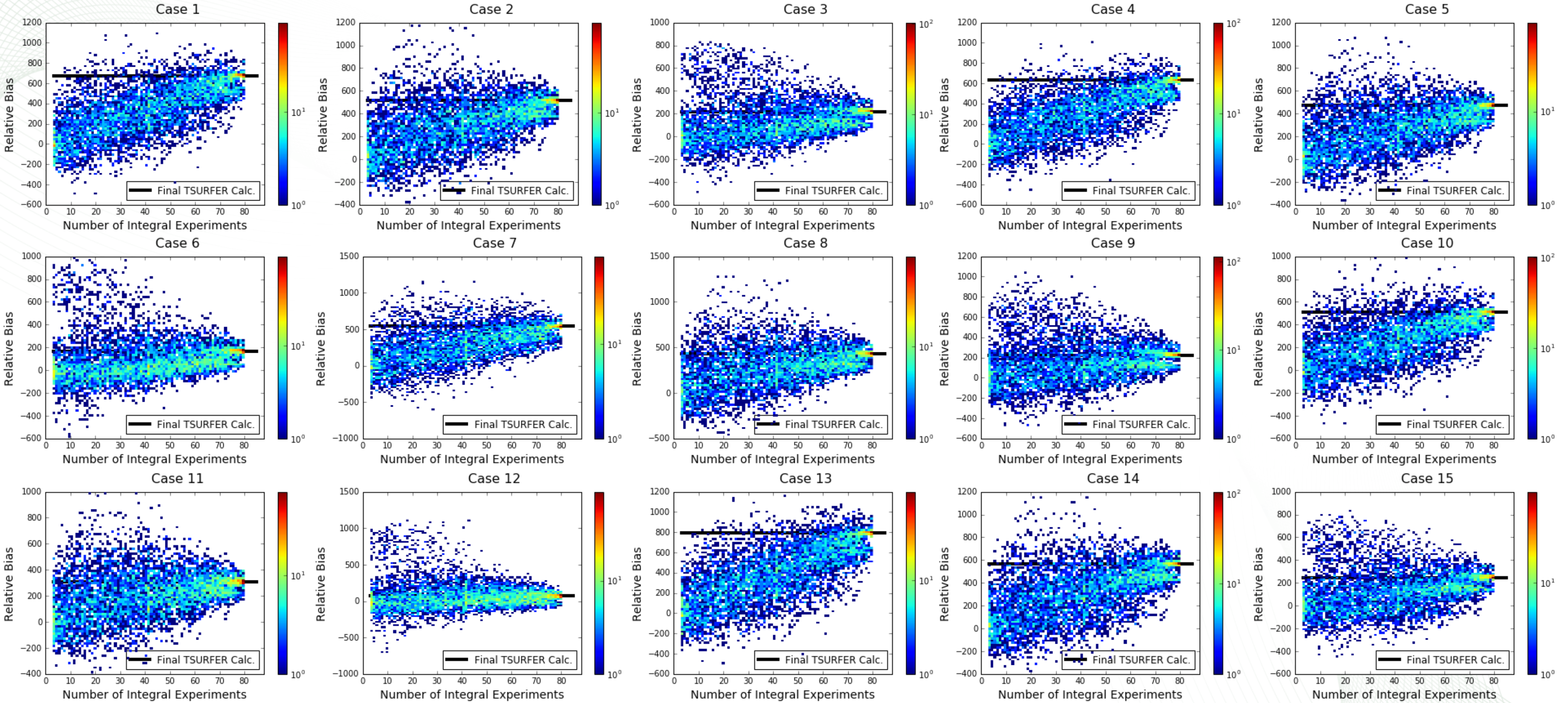
➔ **Examine the convergence of the data-induced uncertainty in the adjusted response.**

➔ **Add more experiments.**

- 25 additional (uncorrelated) experiments were modeled using sample inputs from the ICSBEP.
  - These inputs do not meet ORNL’s VALID Library’s rigorous QA standards.

Results – 56-group Covariance, 81 Exp.



Is the TSURFER solution under-constrained?

- Some differences exist between the 56-experiment and 81-experiment TSURFER simulations.
- It's difficult to tell if the 81-experiment simulation is:
  - Converging to a better value because of its additional experiments; or
  - Converging to a worse value because of its lower fidelity models.

➔ TSURFER biases did not vary greatly with the addition of additional, lower fidelity experimental results.

56-group covariance library

Relative Biases

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9	Case 10	Case 11	Case 12	Case 13	Case 14	Case 15
56 Exp.	576	601	342	568	571	281	599	639	403	467	481	262	649	608	340
81 Exp.	676	516	218	630	472	167	539	429	223	509	309	70	794	568	246

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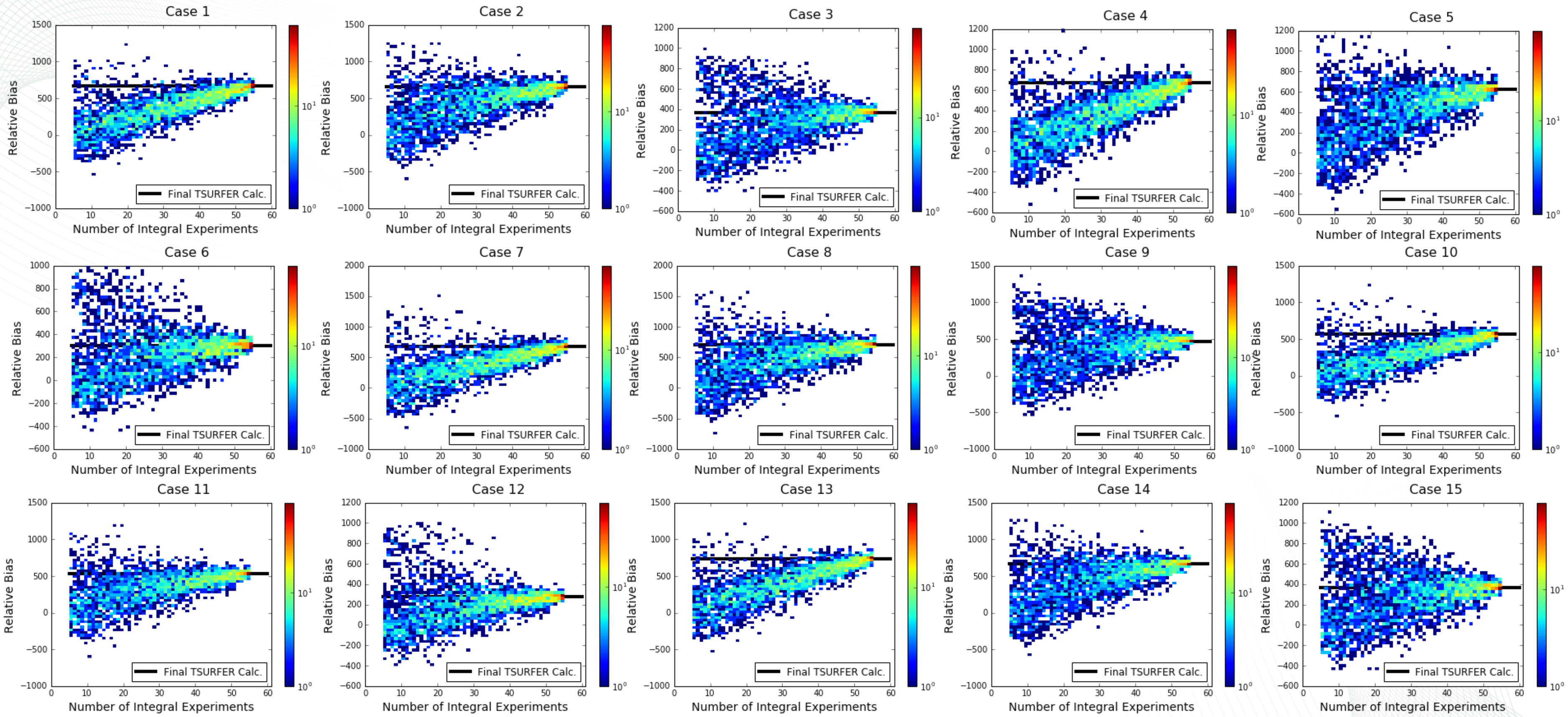
Challenges for Data Assimilation

4. Is the covariance data accurate, or at least “good enough” ?

➔ **Let’s examine results using 44-group covariance data.**

Results – 44-group Covariance, 56 Exp.



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56-group covariance library
44-group covariance library

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56 Exp.	576 664	601 651	342 366	568 673	571 625	281 301	599 674	639 703	403 469	467 564	481 529	262 274	649 737	608 662	340 364
81 Exp.	676 678	516 645	218 412	630 696	472 641	167 387	539 662	429 636	223 453	509 525	309 443	70 239	794 788	568 700	246 454

➔ **Results from different covariance data libraries are generally consistent.**

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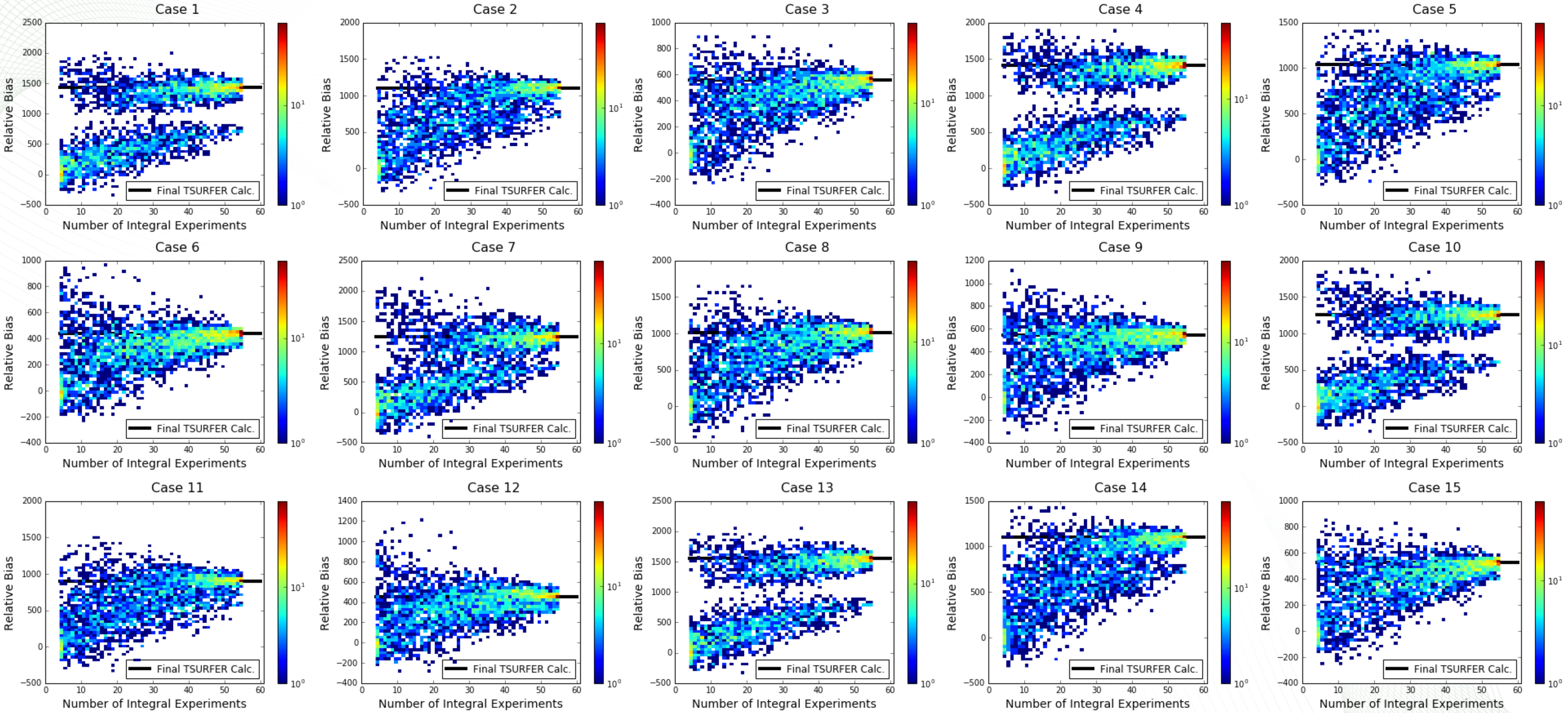
Challenges for Data Assimilation

1. Are any of the experiments outliers or erroneous? (Part II)

➔ **Delta Chi-squared filtering used to detect inconsistent experiments.**

Results – 56-group Cov., 56 Exp., No Chi^2 Filtering



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56-group covariance library
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No Exp. Filtering	1,433 1,122	1,102 863	559 449	1,412 1,154	1,035 854	439 397	1,246 1,107	1,011 873	543 505	1,253 967	896 644	452 298	1,548 1,231	1,099 899	526 448

➔ **Inconsistent experiment filtering matters!!**

Challenges for Data Assimilation

5. How do we get a 95/95 confidence interval from these results?

➔ **Similar to the Whisper method, a margin of subcriticality can be defined:**

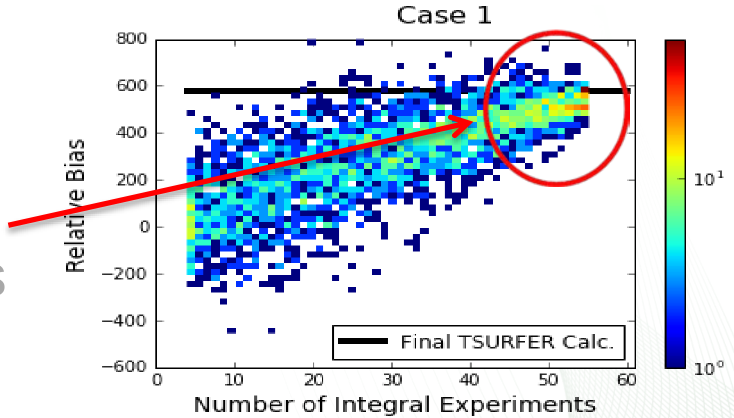
$$MOS = MOS_{software} + MOS_{data} + MOS_{TSURFER}$$

Estimating TSURFER Confidence Intervals

- To determine MOS_{data}, a 95/95 confidence interval is calculated for a normal distribution where:

$$\mu = \min(\,0, -\text{TSURFER-predicted bias}\,)$$
$$\sigma = \text{The TSURFER-adjusted response uncertainty}$$

- The $MOS_{TSURFER}$ is determined by evaluating a non-parametric 95/95 confidence interval around the randomly sampled TSURFER results as they converge to a bias estimate.



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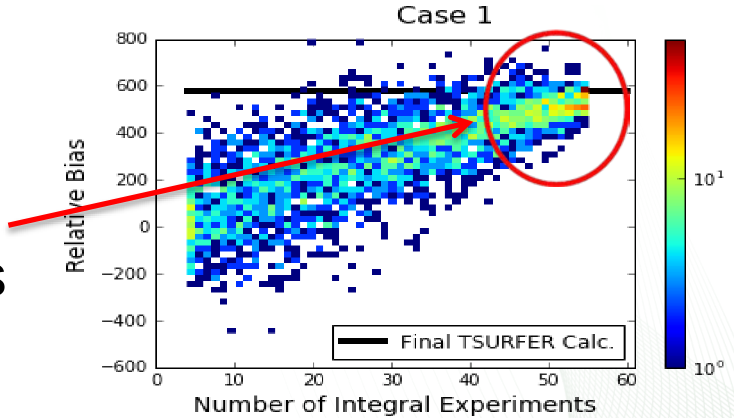
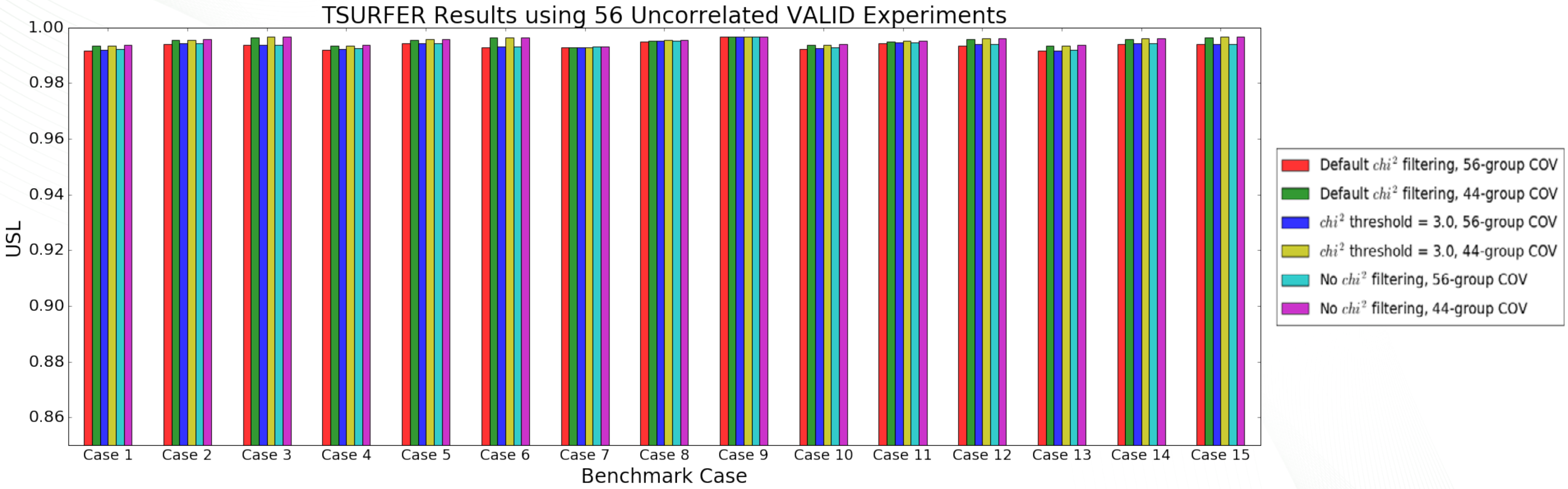


USL Results: Unknown Bias Cases TSURFER Data Assimilation Analysis



Max c_k	0.6935	0.6627	0.837	0.6760	0.6822	0.8347	0.7753	0.7194	0.9293	0.729	0.6683	0.8649	0.6566	0.6716	0.7950
Cases w/ $c_k > 0.9$	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0

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Estimating TSURFER Confidence Intervals

- TSURFER USL estimates were significantly closer to 1.0 than all other USL estimates.
  - TSURFER also predicted a positive bias ($k_{calc} > k_{actual}$) for all application experiments.
- The 44-group covariance data calculations produced smaller $\mathrm{MOS}_{\mathrm{TSURFER}}$ estimates because their bias convergence plots produced less noise.

Conclusions

- By randomly omitting different numbers of experiments, it was generally easy to see when TSURFER calculations failed to converge, or converged to a bad results.
- TSURFER bias estimates for the unknown bias cases could benefit from additional critical experiments.
- Filtering inconsistent experiments is important for trending analysis, data assimilation, and Whisper methods.
  - Note: the Whisper method also utilizes TSURFER post-adjustment uncertainties.

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