Estimating Computational Biases for Criticality Safety Applications with Few Neutronically Similar Benchmarks

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Introduction

- Criticality safety analyses rely on the availability of relevant benchmark experiments to determine justifiable margins of subcriticality.
- Validation efforts seek use benchmark experiments to estimate the computational bias in the predicted eigenvalue for applications.

$$Bias = \beta = k_{calc} - k_{exp}$$

Introduction

- This study is meant to compare the predictive capabilities of criticality safety validation approaches.
- This blind benchmark study applies predictive capabilities to low-moderated MOX powder experiments with few representative experiments.
  - This study was also performed using 10 cases with known biases.

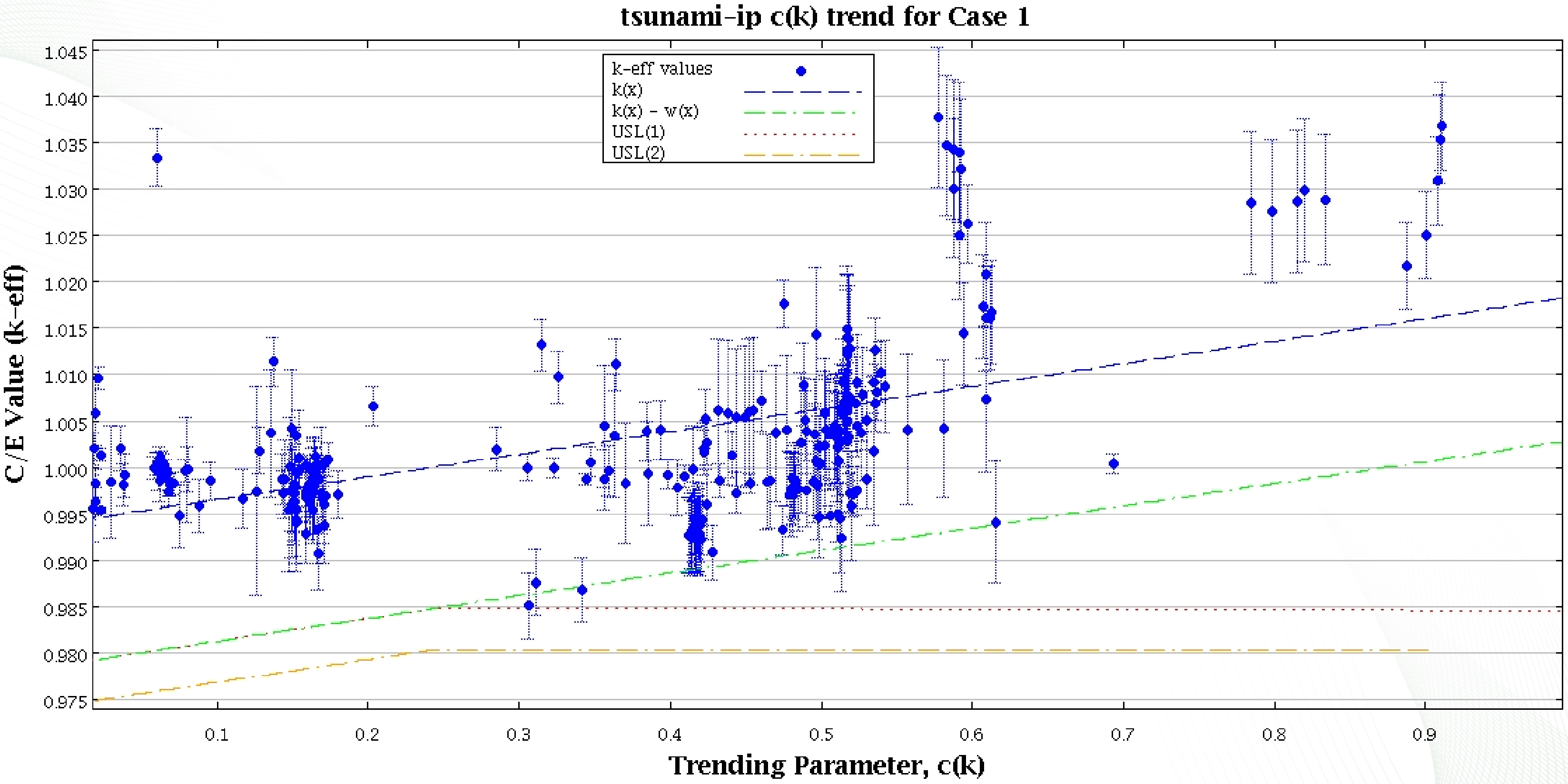
Introduction

- Our study compares three bias estimation methodologies:
  - Trending Analysis (USLSTATS, ORNL)
  - Non-parametric Methods (Whisper, LANL)
  - Experimental Data Assimilation (TSURFER, ORNL)

Trending Analysis – USLSTATS

- USLSTATS is a generic parameter trending analysis tool from ORNL.
- USLSTATS provides several predictive confidence parameters, including:
  1. Expected application bias
  2. Confidence band with administrative margin (USL1)
     - Does not give credit for positive biases.
  3. Single-sided, uniform-width confidence interval (USL2)
- The administrative margin was set to zero for this exercise for all methods.

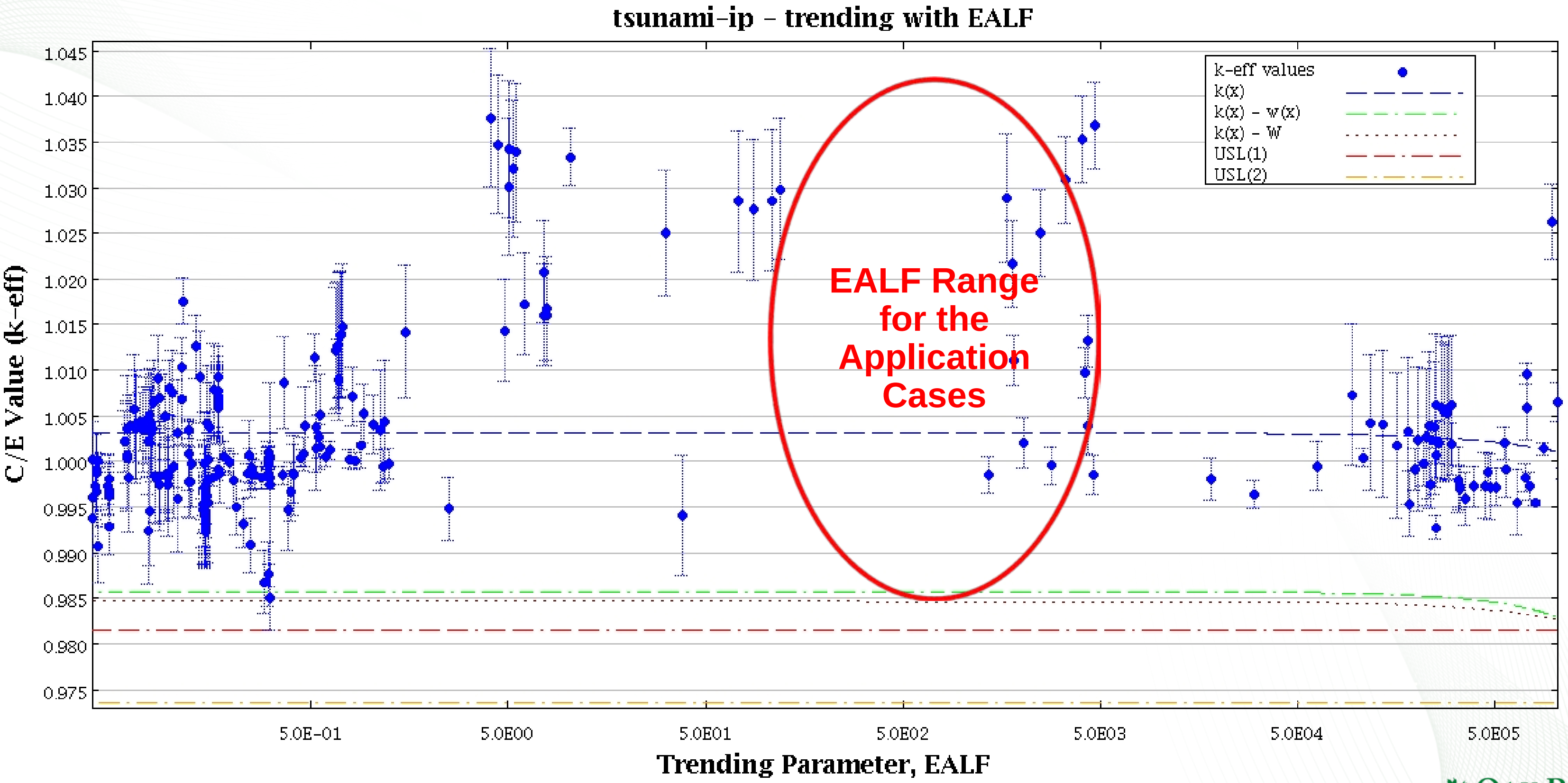
Trending Analysis – Sample USLSTATS Output



Trending Analysis – USLSTATS

- Trending parameters examined in this study included:
  1. The coefficient of similarity, c(k) or c_k
  2. The Energy of the Average Lethargy of Fission (EALF)
- Since the UACSA Phase V exercise is a blind benchmark study, we don’t know for sure what the correct answer is.
  – Cases with known biases were examined to explore the accuracy of the bias estimation methods.
  – For the unknown bias cases, emphasis will be placed on methods that produce consistent results.

Trending on EALF



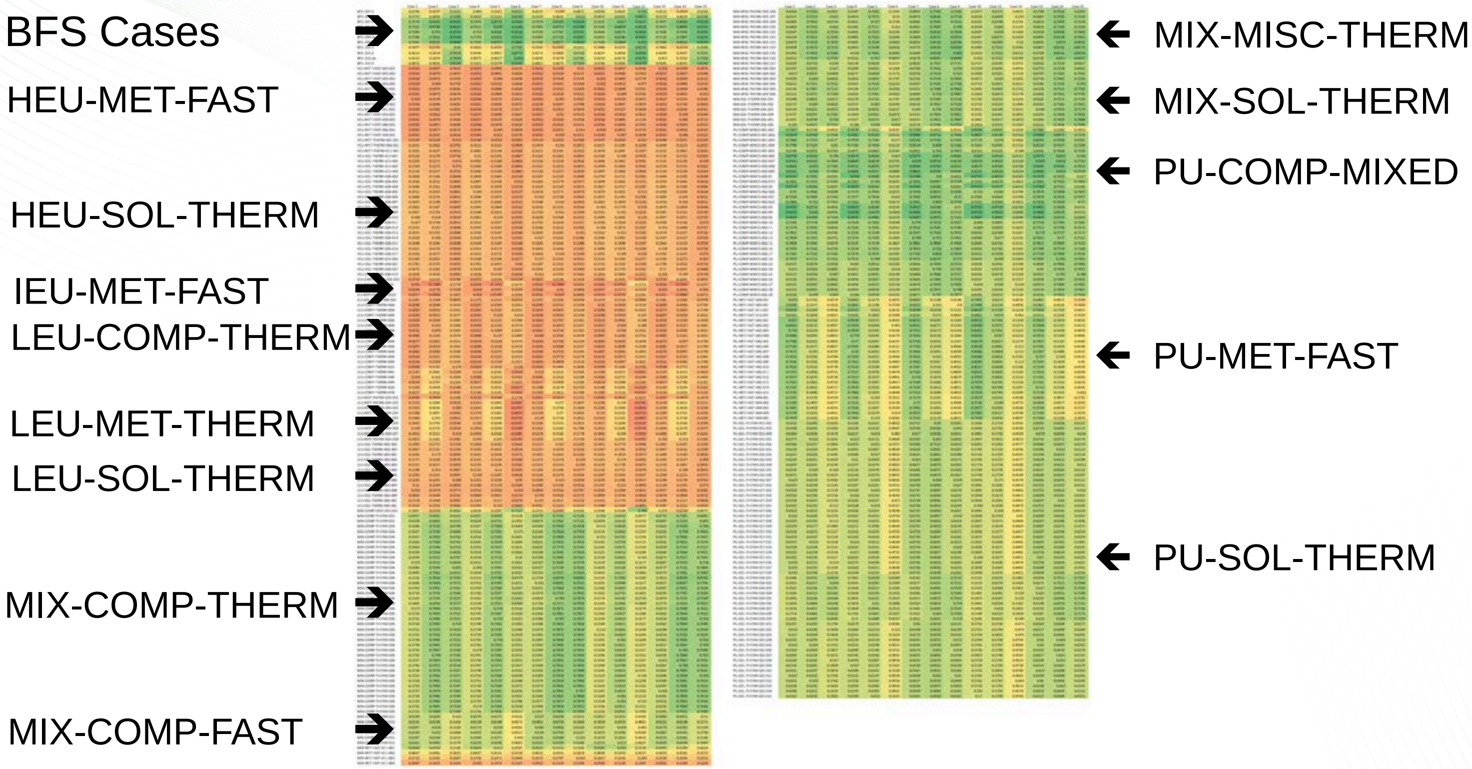
Benchmark Similarity Assessment

- The similarity coefficient, *c(k)* or c_k, describes the amount of nuclear data-induced uncertainty that is shared by two systems.

$$\underbrace{S_{R_1,\Sigma_x}}_{\left(\frac{\delta R/R}{\delta\Sigma/\Sigma}\right)} \cdot \underbrace{Cov_{\Sigma_x,\Sigma_y}}_{(\Delta\Sigma/\Sigma)^2} \cdot \underbrace{S^T_{R_2,\Sigma_y}}_{\left(\frac{\delta R/R}{\delta\Sigma/\Sigma}\right)} = \underbrace{\sigma^2_{R_1,R_2}}_{(\Delta R/R)^2}$$

$$c_k = \frac{\sigma^2_{R_1,R_2}}{\sigma_{R_1}\sigma_{R_2}}$$

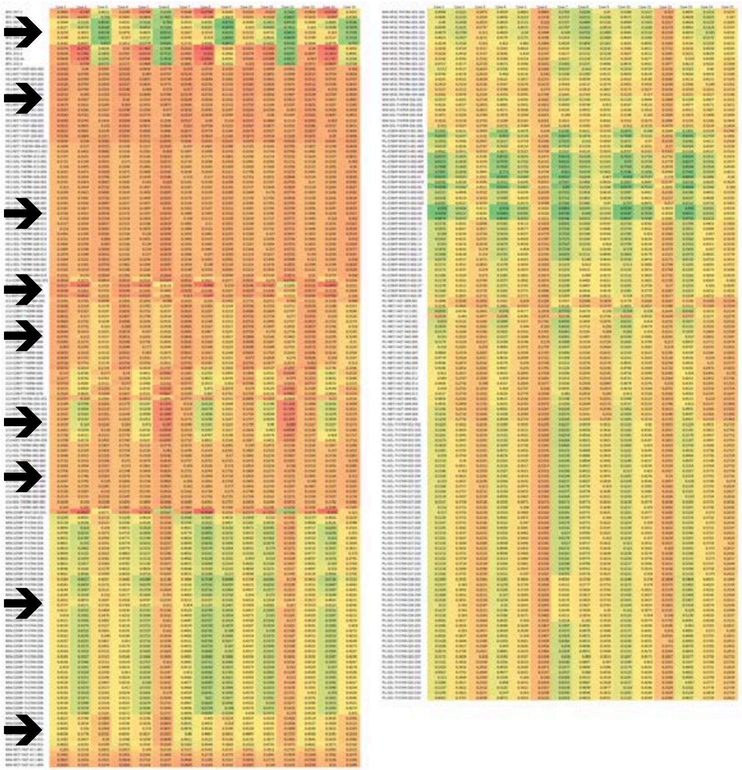
Benchmark Experiment Similarity Coefficients – 44-group Covariance Data



c(k) Color Key
1.0
0.8
0.6
0.4
0.2
0.0
-0.2

Benchmark Experiment Similarity Coefficients – 56-group Covariance Data

BFS Cases →
HEU-MET-FAST →
HEU-SOL-THERM →
IEU-MET-FAST →
LEU-COMP-THERM →
LEU-MET-THERM →
LEU-SOL-THERM →
MIX-COMP-THERM →
MIX-COMP-FAST →



← MIX-MISC-THERM
← MIX-SOL-THERM
← PU-COMP-MIXED
← PU-MET-FAST
← PU-SOL-THERM

c(k) Color Key
1.0
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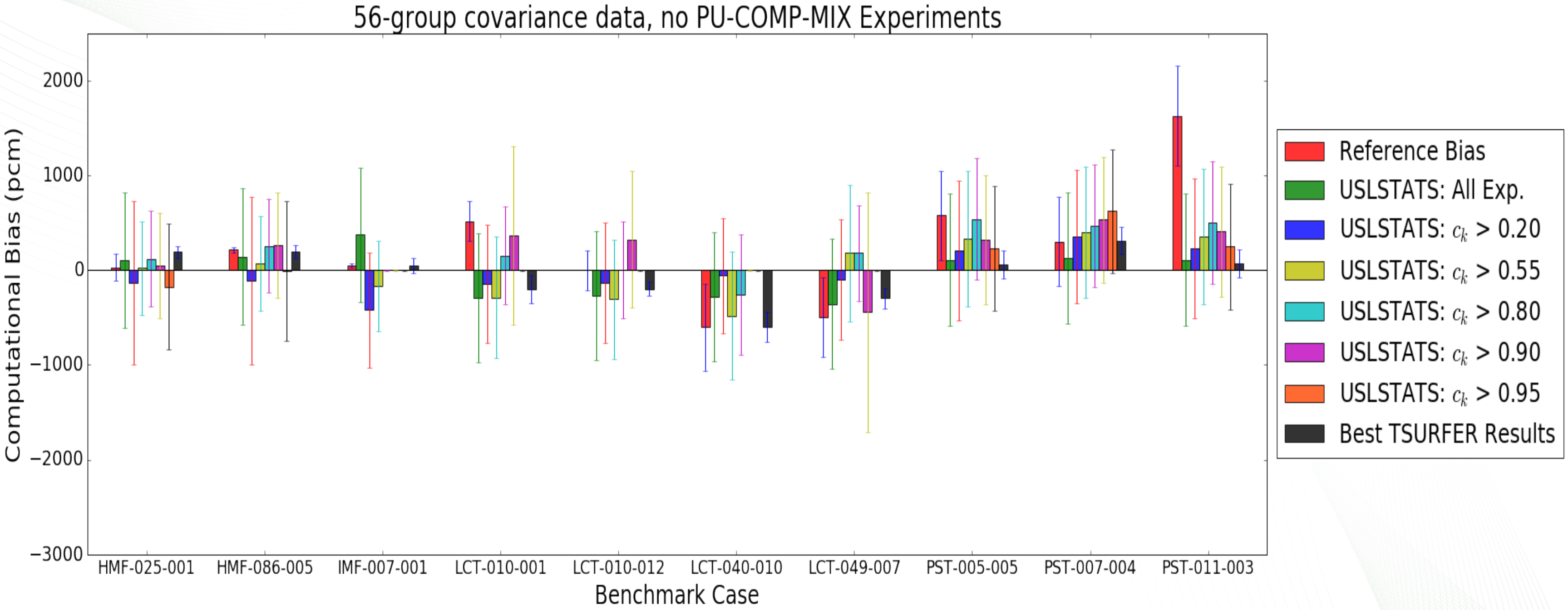
Bias Results: Known Bias Cases USLSTATS c_k Trending Analysis



Max c_k	0.9986	0.9962	0.9642	0.9674	0.9694	0.9527	0.9766	0.9998	0.9999	0.9982
Cases with $c_k > 0.9$	14	14	1	10	16	2	4	55	56	55

USLSTATS Results – Takeaways:

< 2 σ Error
2-3 σ Error
> 3 σ Error

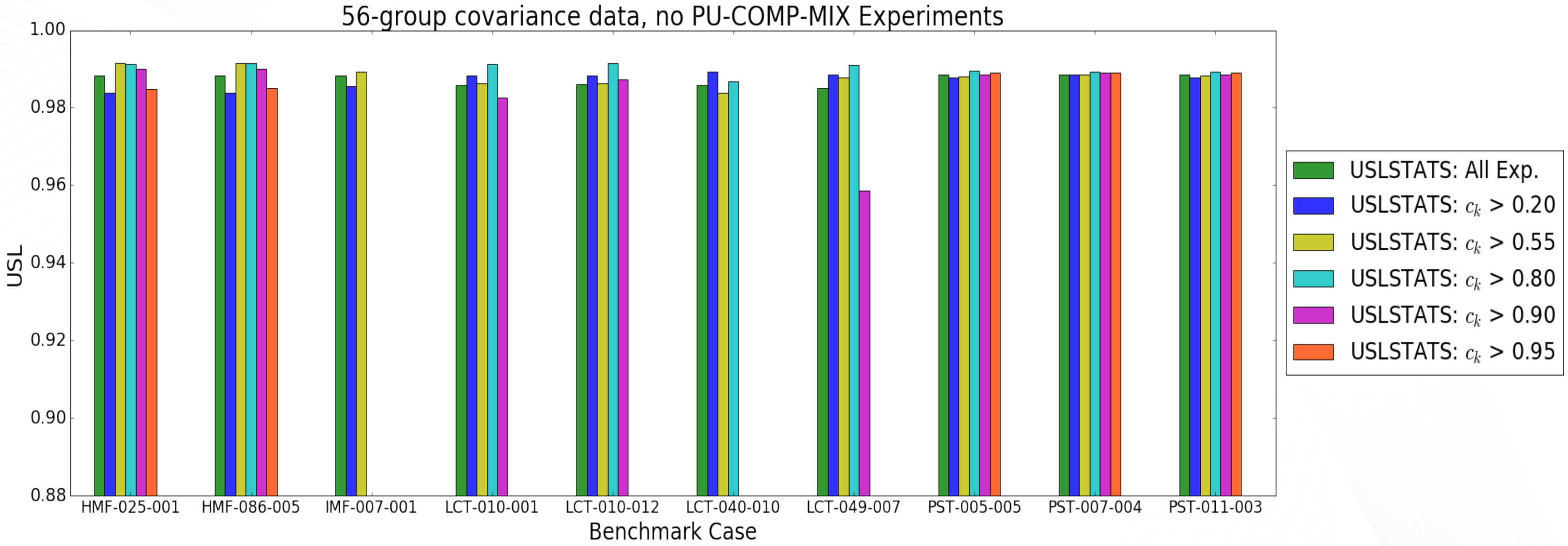
	Difference (Units of σ)	All Exp.	c_k > 0.2	c_k > 0.65 c_k > 0.55	c_k > 0.8	c_k > 0.9	c_k > 0.95	Best TSURFER Results
44-group Covariance Data	**Average**	**3.43**	**11.72**	**3.03**	**1.26***	**1.10***	**4.54***	**1.56**
	Max	**8.36**	**35.98**	**8.24**	**2.38***	**2.44***	**9.11***	**3.38**
56-group Covariance Data	**Average**	**5.23**	**7.93**	**3.86**	**1.20***	**1.17***	**3.46***	
	Max	**15.55**	**22.27**	**10.11**	**2.12***	**2.31***	**7.06***	

* Too few cases existed to compute bias estimates for at least one application.

USLSTATS Results – Takeaways:

- USLSTATS predicted accurate computational biases when enough high similarity benchmark experiments were present.
- The “best” USLSTATS bias predictions were more accurate than the “best” TSURFER bias predictions.
- This comparison could be strengthened if the benchmark experiment results had smaller error bars.

USL Results: Known Bias Cases USLSTATS c_k Trending Analysis



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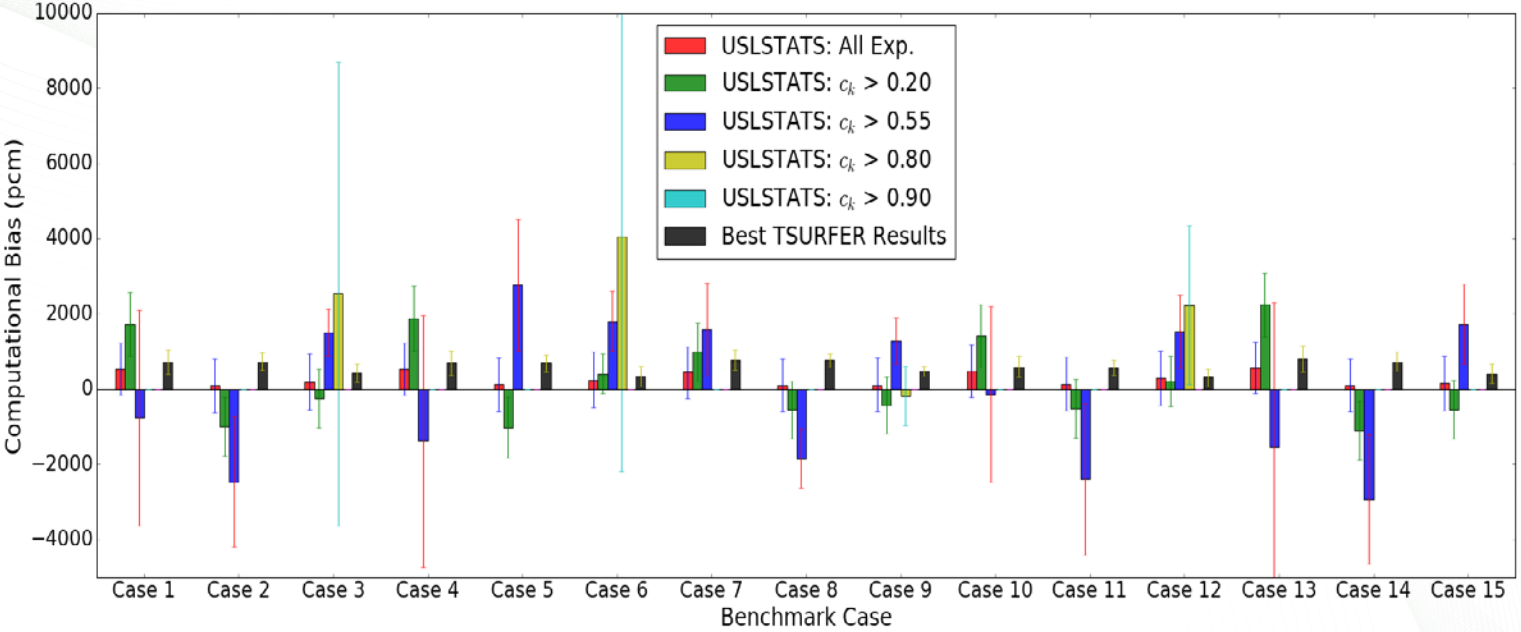
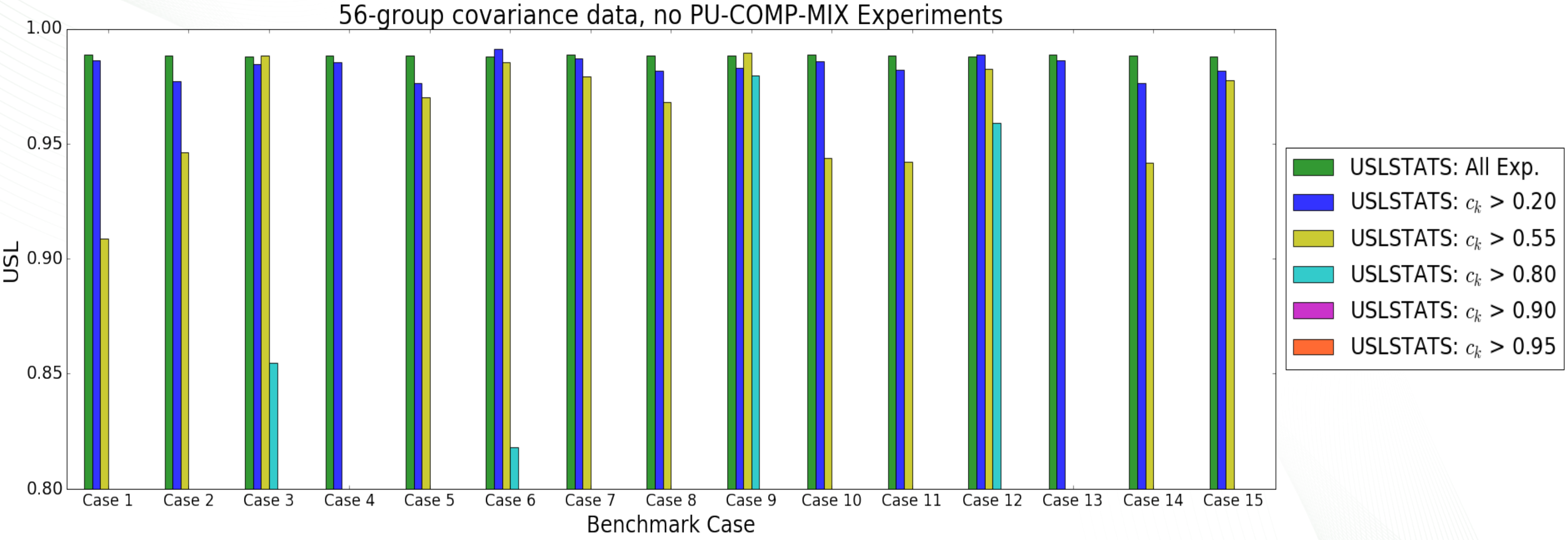


Max c_k	0.6935	0.6627	0.8370	0.6760	0.6822	0.8347	0.7753	0.7194	0.9293	0.7290	0.6683	0.8649	0.6566	0.6716	0.7950
Cases w/ $c_k > 0.9$	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0

USL Results: Unknown Bias Cases USLSTATS c_k Trending Analysis



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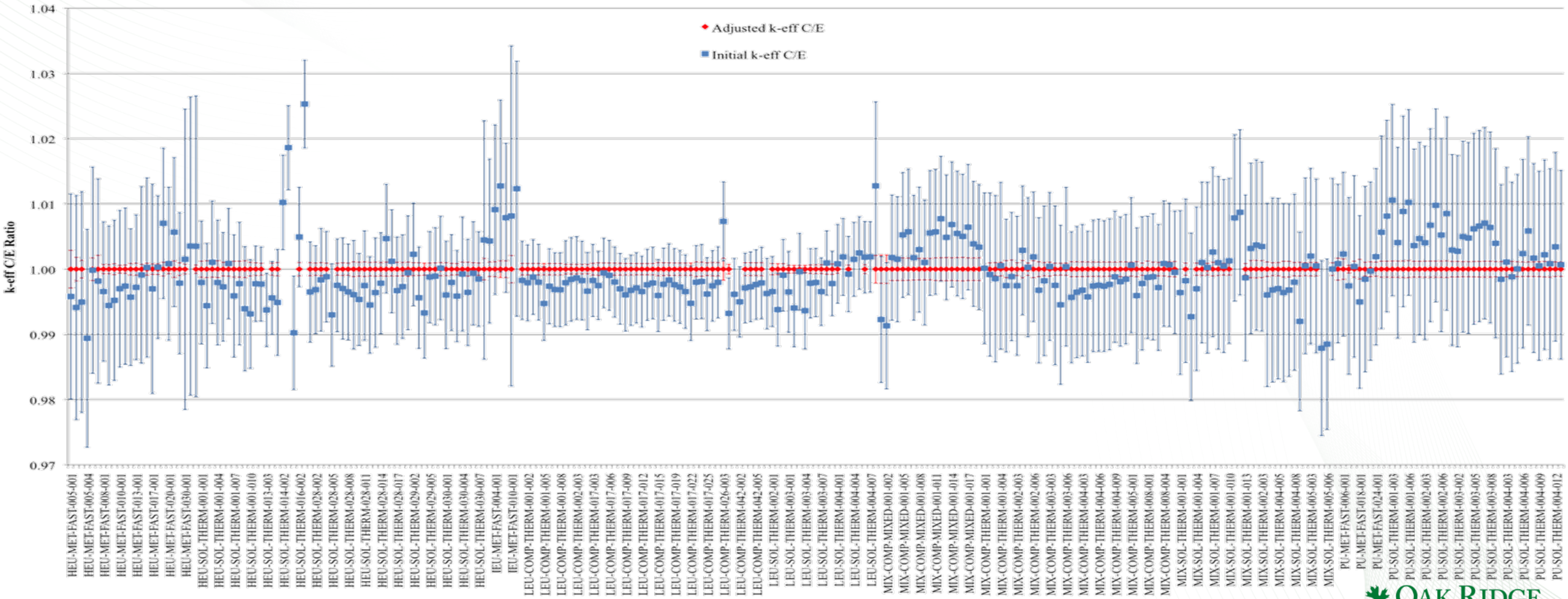
TSURFER Tools for Data Adjustment and Experimental Data Assimilation

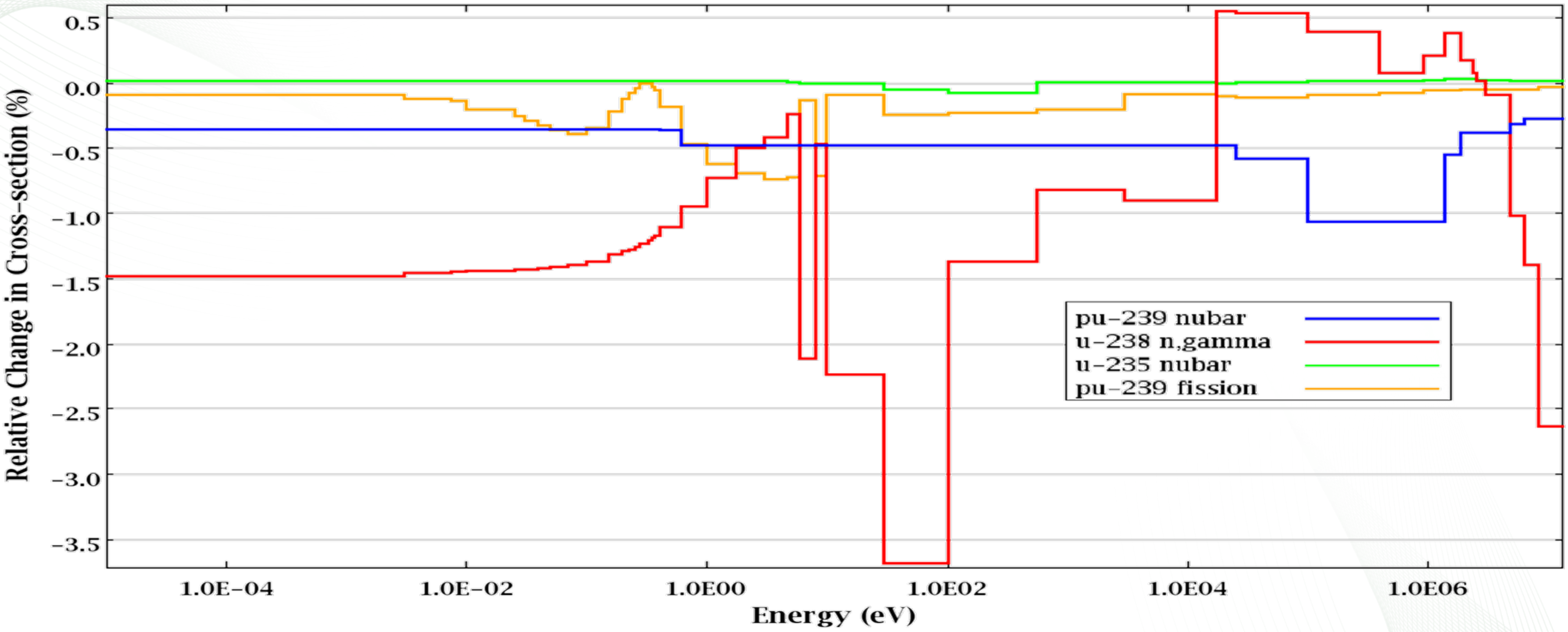
- *TSURFER:* *T*ool for *S*/*U* analysis of *R*esponse *F*unctionals using *E*xperimental *R*esults
  - Biases are observed as differences between benchmark and computed quantities (k_{eff}, reaction rates, etc.)
  - TSURFER uses sensitivity information to **consistently** adjust nuclear data and reconcile biases between integral experiment results and computational predictions.
  - Where the cross sections and covariance data are modified, the modifications can be used to project biases from the benchmarks to targeted application systems.

Data Adjustment Techniques:

Experimental benchmark data (E) is used to improve the accuracy of the initial computed responses (C).



TSURFER Cross Section Adjustments



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A Note on Bias

- The computational bias measures the predictive capabilities of a modeling and simulation tool.
- For USLSTATS:

$$Relative\ Bias = C/E_{Extrapolated} - 1$$

- For TSURFER:

$$Relative\ Bias = \frac{(Calculated\ Response\ - Adjusted\ Response)}{Calculated\ Response}$$

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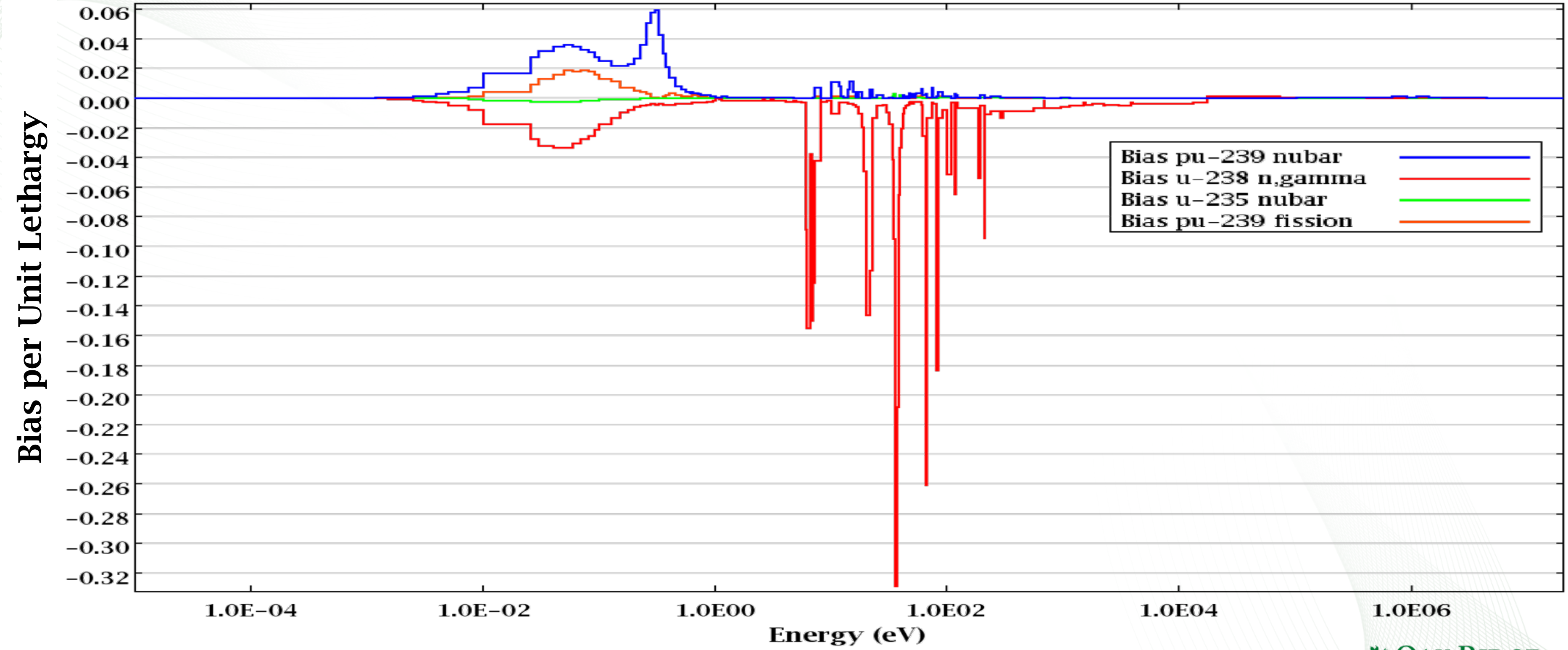
Bias Estimation

$$\textbf{Bias} = k_{\text{Simulation}} - k_{\text{Experiment}}$$



Adjusted Cross Sections Reduce Data-Induced Biases

- Original Application Uncertainty is:
  0.520% Δk/k

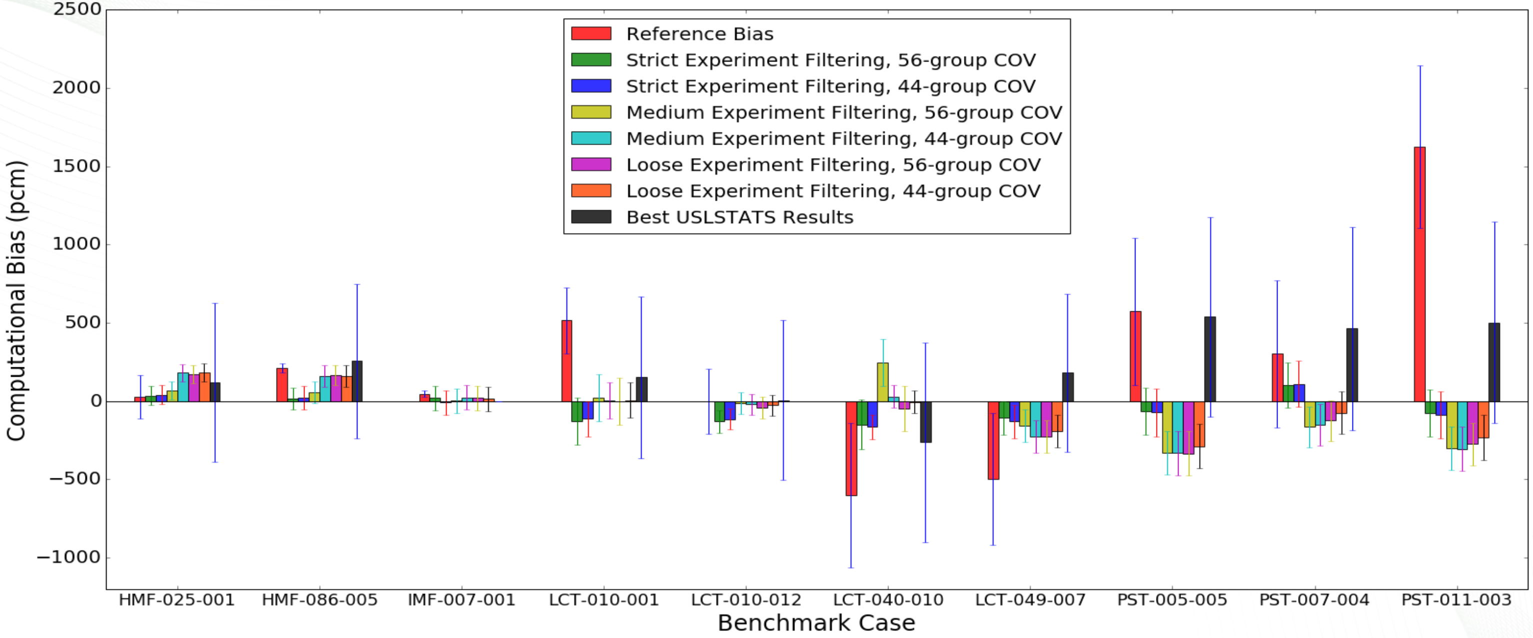
- Adjusted Application Uncertainty is:
  0.119% Δk/k

- Interpretation: ~80% of uncertainty is quantified through validation with experiments.

- Remaining uncertainty highlights gaps in available validation data.

NUCLIDE	REACTION	CONTRIBUTION TO BIAS % dk/k
u-238	n,gamma	-2.1084E-01
pu-239	nubar	1.2761E-01
pu-239	fission	3.9872E-02
o-16	elastic	3.2243E-02
pu-239	n,gamma	-2.5810E-02
pu-239	chi	1.0248E-02
u-235	chi	2.9940E-04
fe-56	n,gamma	1.7158E-02
u-235	fission	-1.2351E-02
pu-240	n,gamma	-1.3162E-02
u-238	elastic	2.7715E-03
u-235	n,gamma	1.0599E-03
h-1	elastic	2.7348E-03
u-238	n,n'	-6.8963E-03
u-235	nubar	-4.1298E-03
fe-56	elastic	-6.0079E-03
h-1	n,gamma	4.1893E-03
u-238	nubar	3.1408E-03

Bias Results: Known Bias Cases TSURFER Analysis



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TSURFER Results – Takeaways:

< 2 σ Error
2-3 σ Error
> 3 σ Error

	Difference (Units of σ)	Strict Filtering	Medium Filtering	Loose Filtering	Best USLSTATS Results
44-group Covariance Data	**Average**	**3.04**	**1.61**	**1.59**	**1.20***
	Max	**-8.13**	**-3.03**	**-3.04**	**2.12***
56-group Covariance Data	**Average**	**3.39**	**1.56**	**1.53**	
	Max	**-9.59**	**-3.38**	**-3.35**	

* Too few cases existed to compute bias estimates for at least one application.

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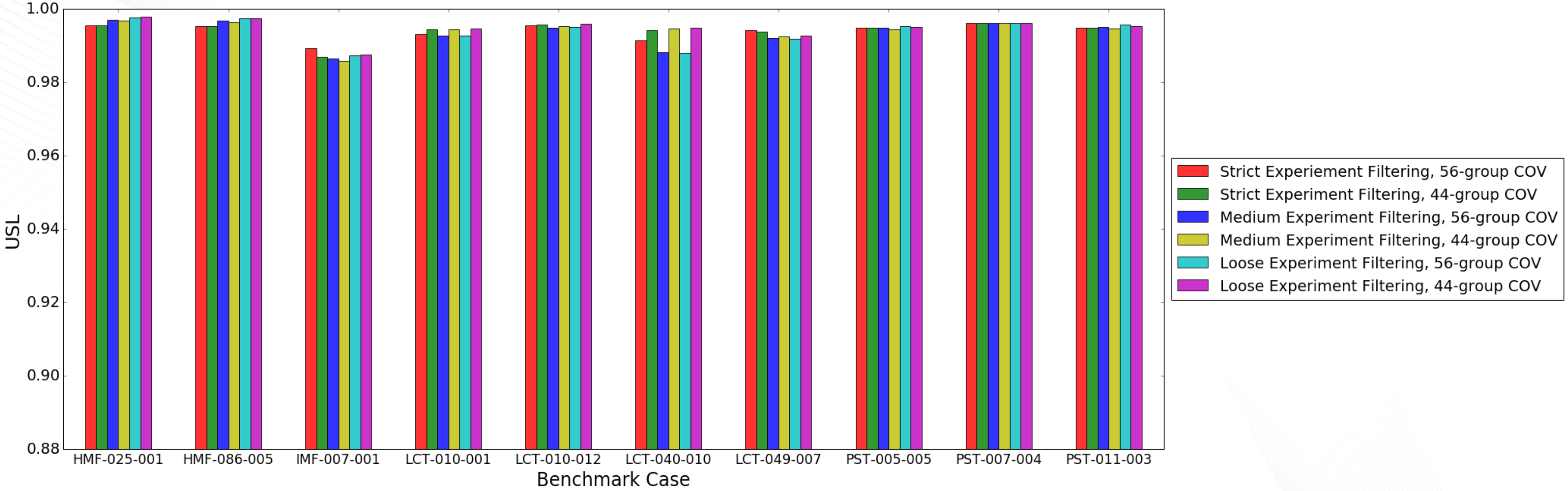
TSURFER Results – Takeaways:

- TSURFER bias predictions were slightly less accurate than the best USLSTATS bias predictions.

- The TSURFER bias predictions were significantly more consistent than the USLSTATS predictions (more discussion about this later).

USL Results: Known Bias Cases TSURFER Analysis



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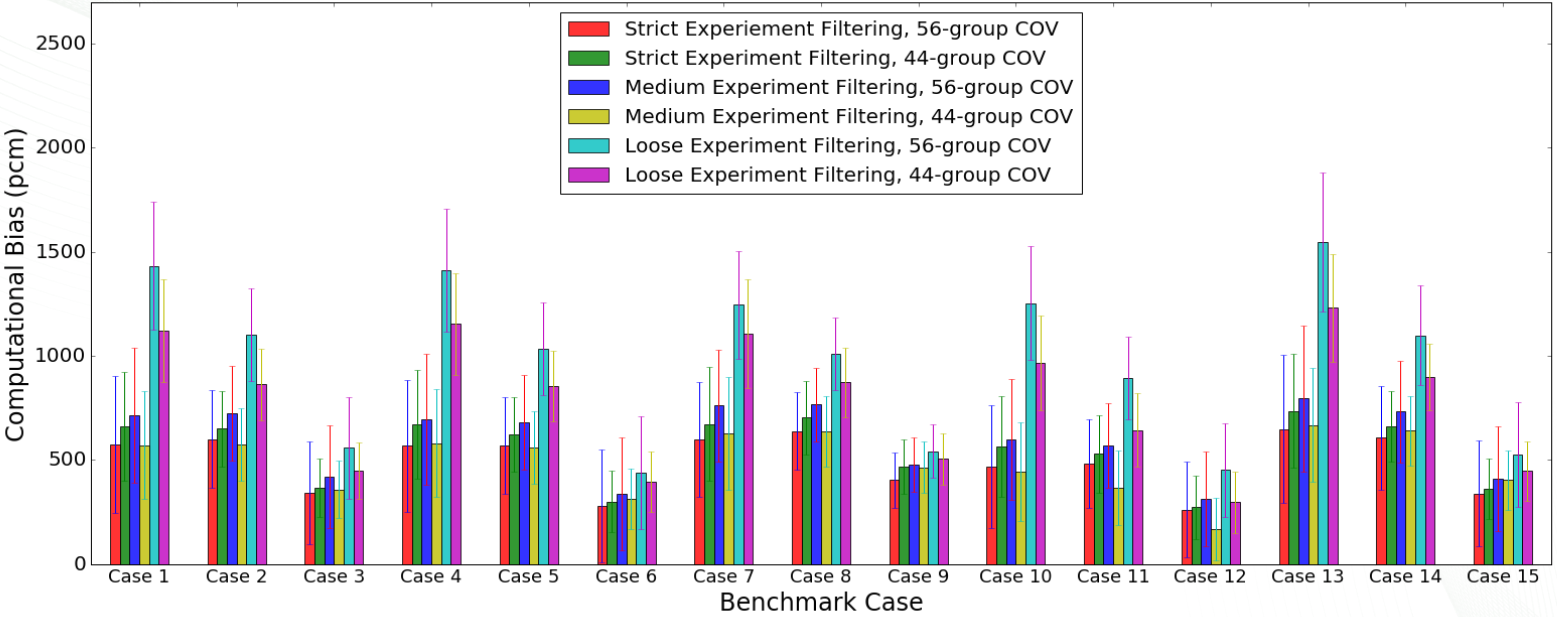
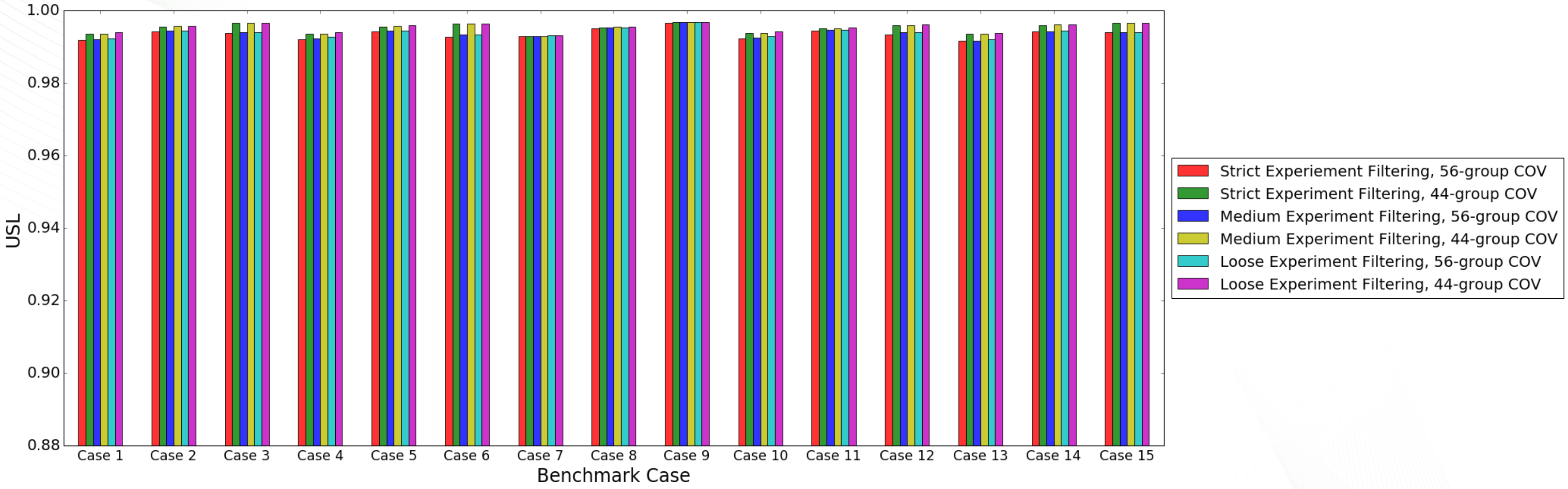
USL Results: Unknown Bias Cases TSURFER Data Assimilation Analysis



Max c_k	0.6935	0.6627	0.8370	0.6760	0.6822	0.8347	0.7753	0.7194	0.9293	0.7290	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

USL Results: Unknown Bias Cases TSURFER Data Assimilation Analysis



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TSURFER Results – Takeaways:

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- The TSURFER bias predictions were significantly more consistent than the USLSTATS predictions (more discussion about this later).
- TSURFER USL estimates are much closer to 1.00 than USLSTATS estimates.

TSURFER: ~0.99 **USLSTATS:** 0.96 – 0.98

Whisper Methodology

- Non-parametric, extreme-value theory based method for determining USL's and margins of subcriticality (MOS).
  - Developed by Kiedrowski at LANL in 2014
- Whisper USL's are designed to be conservative.
  - Adding more benchmark cases can only increase the MOS.
- Results presented here were obtained using an independently-developed implementation of the Whisper methodology.

Whisper Methodology

- Whisper weights the importance of experiments based on their similarity to the target application.

$$weight_i = \frac{\left(c_k^i - c_k^{threshold}\right)}{\left(\max(c_k) - c_k^{threshold}\right)}$$

- Whisper includes additional benchmark experiments until a cumulative weight of 25 is obtained.
  - Treatments exist for applying the Whisper method to cases with few similar benchmarks.

Whisper Methodology

- Whisper uses data assimilation methods to identify inconsistent benchmark experiments and omit them from the USL calculation.
- Whisper uses the adjusted response uncertainty to provide additional subcritical margin.
  - Performing a convergence study on the adjusted response uncertainty is helpful for Whisper analyses.

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

- A detailed discussion of the Whisper methodology is available in:

B.C. Kiedrowski, et. al., "Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Baseline Upper Subcritical Limits," *Nucl. Sci. Eng.* (2015).

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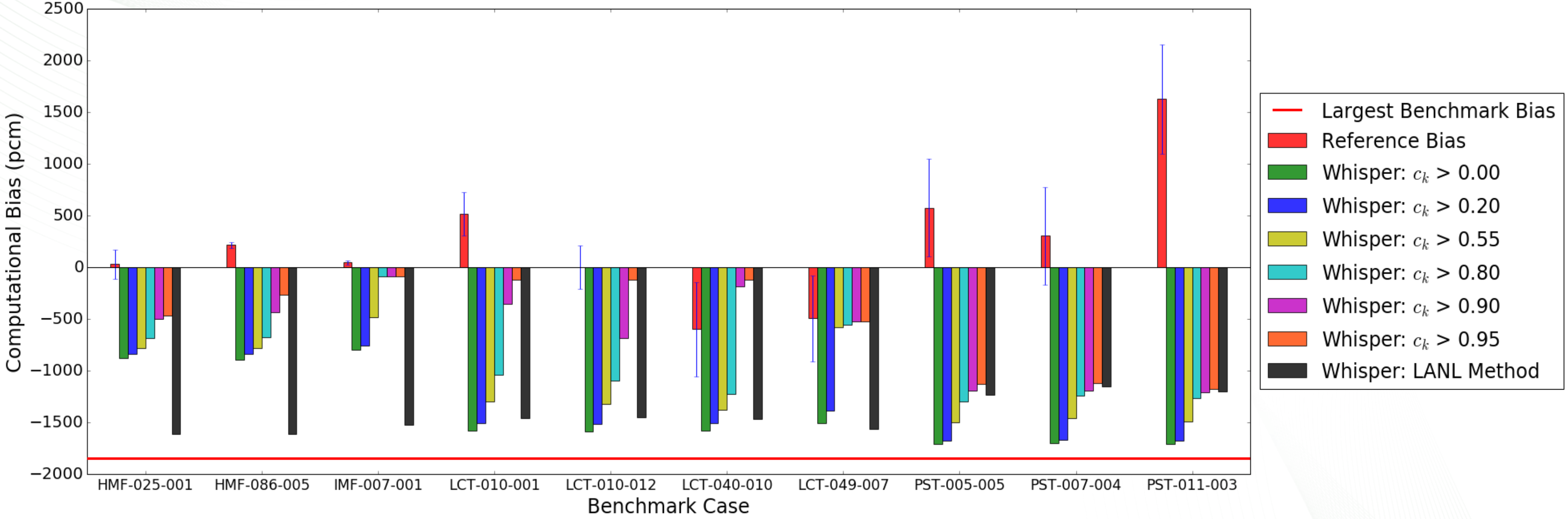
Bias Results: Known Bias Cases Whisper Implementation Analysis



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Whisper Results – Takeaways:

- Whisper bias estimates should be interpreted differently than USLSTATS or TSURFER bias estimates.
- When few highly similar experiments exist, the Whisper bias approaches the bias of the most conservative experiment available.
- As the c_k threshold decreases, the Whisper bias approaches the bias of the most conservative experiment available.

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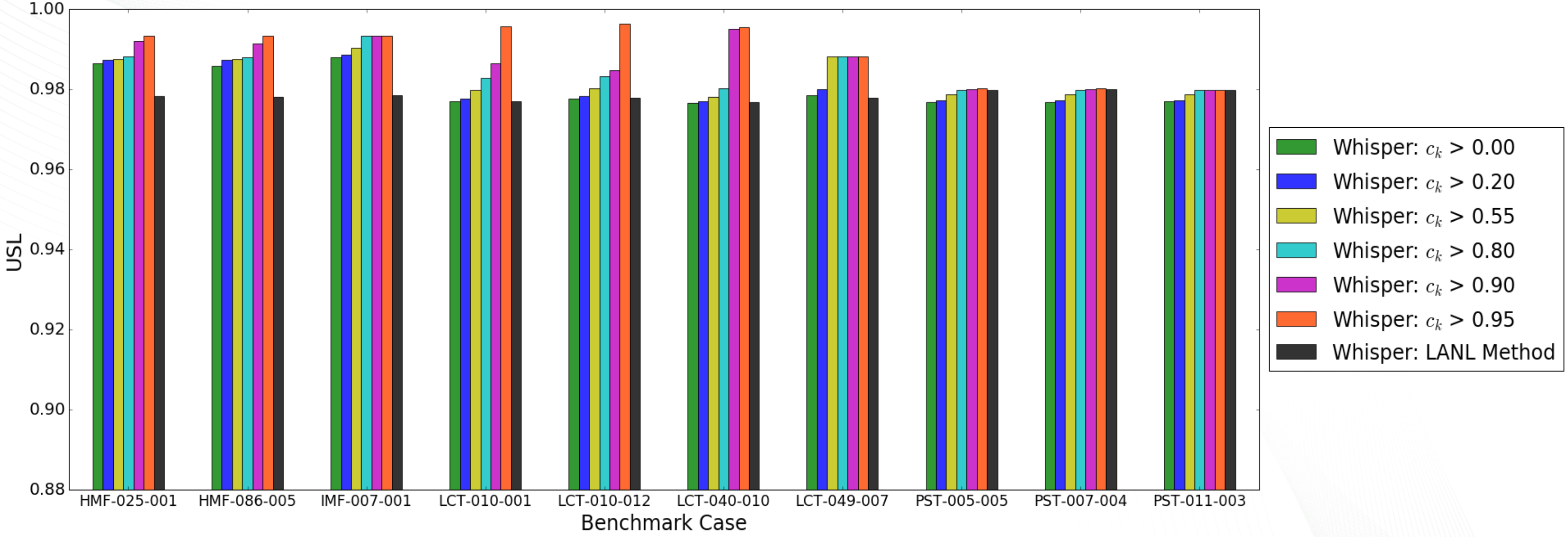
USL Results: Known Bias Cases Whisper Implementation Analysis



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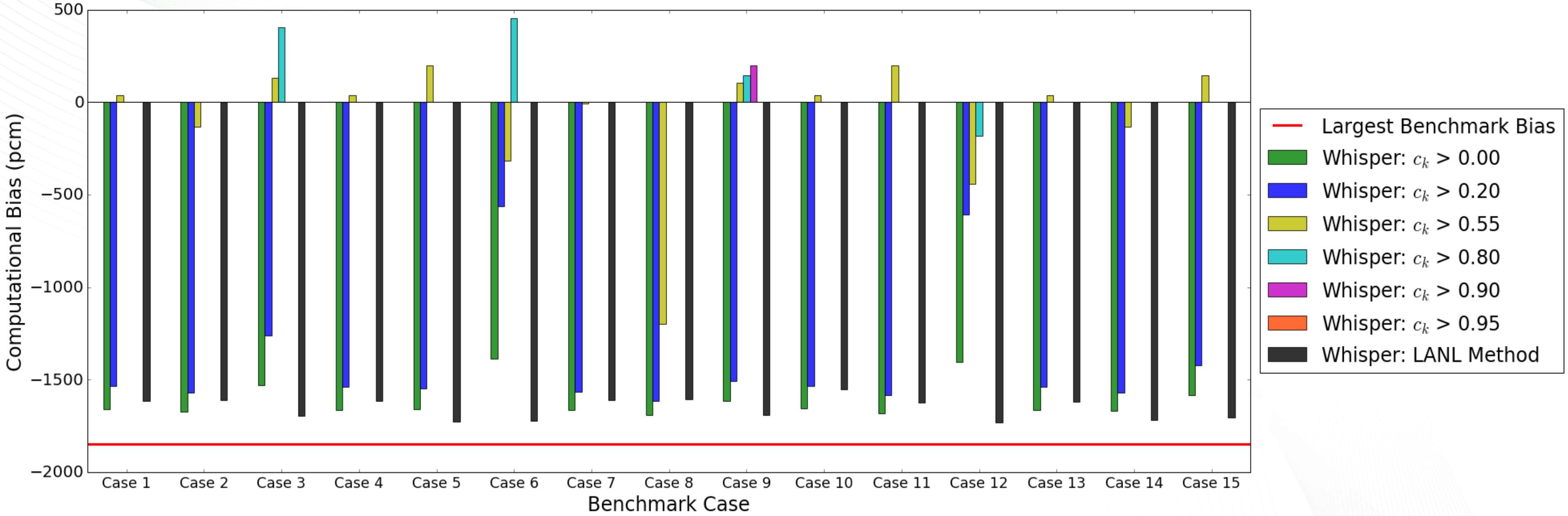
Bias Results: Unknown Bias Cases Whisper Implementation Analysis



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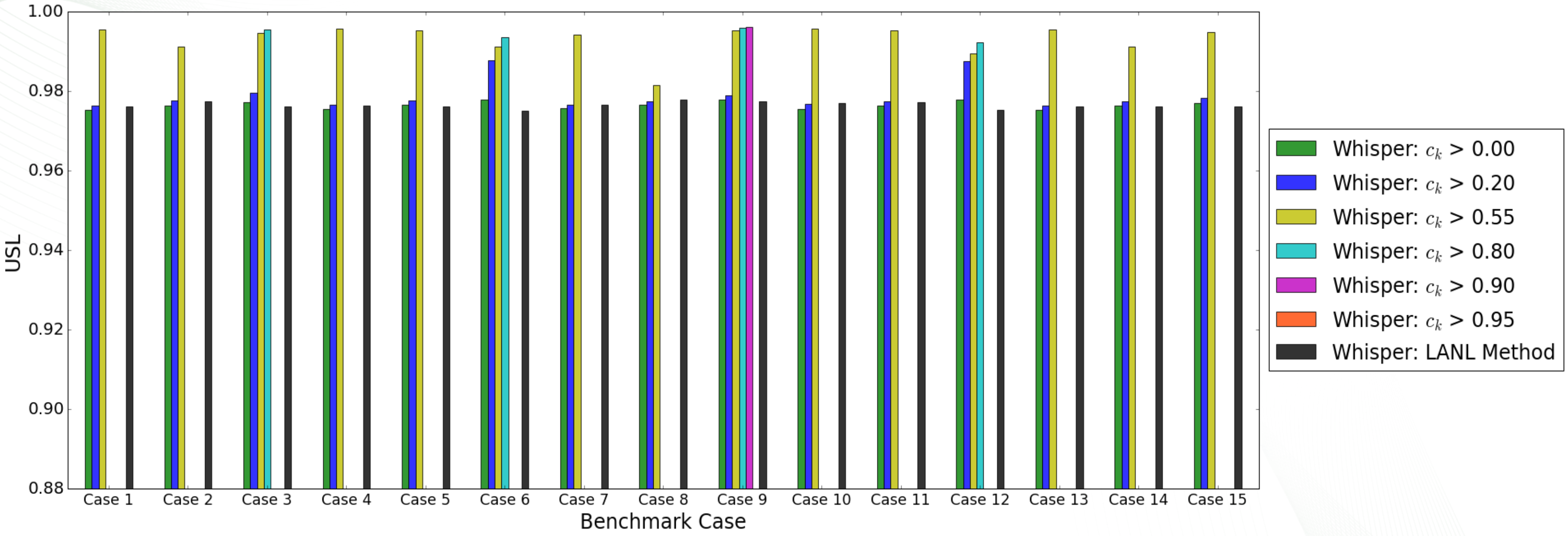
USL Results: Unknown Bias Cases
Whisper Implementation Analysis



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Standard Deviation of Bias Estimates

Covariance Data	Application Cases	USLSTATS	TSURFER (all cases)	TSURFER (cases with filtering)	Whisper (all cases)	Whisper (cases with at least w_i)
44-group	Phase I	361	121	122	441	168
	Phase V	767	162	81	802	50
56-group	Phase I	231	169	166	455	172
	Phase V	1,338	240	101	819	110
Overall	Phase I	295	142	136	434	173
	Phase V	1,020	199	87	1,167	88

* Standard deviations expressed in units of pcm.

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Standard Deviation of USL Estimates

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44-group	Phase I	1,423	115	119	481	115
	Phase V	7,554	61	65	773	70
56-group	Phase I	522	140	137	504	117
	Phase V	4,628	77	83	806	79
Overall	Phase I	1,088	140	145	485	120
	Phase V	6,431	121	114	771	79

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TSURFER Results – Takeaways:

- USLSTATS bias and USL estimates can vary significantly based on the user's input parameters and choice of benchmark experiments.

- The TSURFER and Whisper bias estimates exhibited the greatest degree of consistency.

Conclusions

- USLSTATS and TSURFER produced accurate bias estimates for cases with known biases.
  - USLSTATS trending analyses were found to be most effective when trending on c_k.
  - Setting a very high c_k threshold CAN decrease the accuracy of USLSTATS.
  - High uncertainty in the known bias reference cases makes it difficult to evaluate the accuracy of the bias prediction methods.
- TSURFER and Whisper produced consistent bias and USL estimates for cases with unknown biases, but USLSTATS did not.
- The TSURFER USL estimates are generally less conservative than those from USLSTATS or Whisper.
  - TSURFER was designed for accurate prediction of bias, not conservative USL estimates.

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