Sandia National Laboratories

SAND2019-4558C

A Bayesian Framework for the Integration of Separate and Integral Effects Validation Data

PRESENTED BY

Nathan W. Porter Postdoctoral Appointee

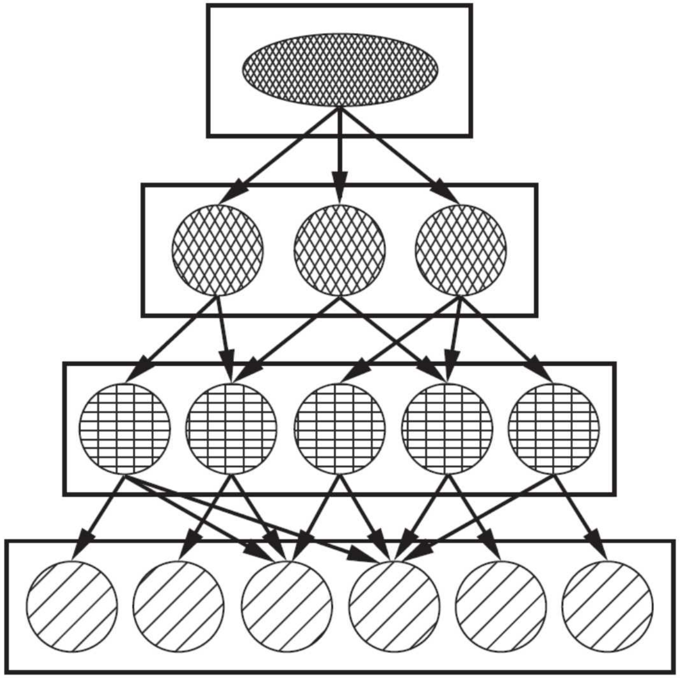
Vincent A. Mousseau Principle Member of the Technical Staff

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

ASME VVS2019-5222

Motivation

- In complex engineering problems, validation can often be subdivided into tiers.
- System, subsystem, benchmark, unit
- Recognizes that the complexity of experiments varies, and that the accuracy and quantity of their data are different.



Demonstration of validation hierarchy[1]

1. Oberkampf, W. L., and Roy, C. J., 2010. Verification and Validation in Scientific Computing. Cambridge University Press. Cambridge, UK. pg. 28.

Background and Theory

Model Calibration, Validation, and Prediction

- After code bugs and numerical errors have been minimized via SQA and verification, the remaining sources of uncertainty must be quantified.
  - Calibration – parameter uncertainty and measurement errors
  - Validation – model form errors
  - Prediction – total uncertainty in the model
- Here, we summarize a methodology which delineates these three processes in a consistent way while utilizing the calibration/validation pyramid.
  1. Set up pyramid
  2. Separate calibration and validation data
  3. Iteratively perform calibration using Bayesian methods
  4. Propagate parameter uncertainty through model for validation cases
  5. Asses validation accuracy and/or predictive capability

Calibration: Statistical Model

- The statistical model generally assumes that the experimental data is equal to some model with zero-mean Gaussian measurement noise.

$$y_d = y_m(x, \theta) + \varepsilon$$

- There are two primary choices for treatment of each parameter.
  1. A purely epistemic parameter has one "true" value which is unknown (e.g., physical constants). The posterior distribution represents epistemic uncertainty in the parameter value.
  2. A parameter may have combined aleatory and epistemic uncertainty. This is treated by assigning the parameter a probability distribution which represents the aleatory uncertainty, then the posterior density represents epistemic uncertainty in the distribution.

- Both methods can employ Bayesian Calibration to obtain estimates of the desired distributions, though they require different likelihood functions.[1]

1. Mullins, J. and Mahadevan, S. 2016. "Bayesian Uncertainty Integration for Model Calibration, Validation, and Prediction." *J Verification Validation UQ*, 1(1).

Calibration: Bayesian Methods

- An approach for statistically inferring unknown parameter values by observing state variables and corresponding data.
- Allows for the incorporation of prior information from previous experiments or expert knowledge.
- Solves Bayes' formula, which formulates the desired posterior distribution in terms of the prior distribution and likelihood function.

$$\pi(\theta|y) = \frac{\mathcal{L}(y|\theta)\pi_o(\theta)}{\int_\Theta \mathcal{L}(y|\theta)\pi_o(\theta)d\theta}$$

- We employ sampling methods because (1) the denominator is difficult or impossible to integrate and (2) the product of the likelihood and prior cannot be easily sampled.

Calibration: Markov Chain Monte Carlo

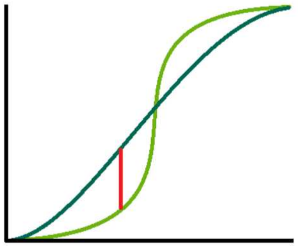
- Methods which construct a sampling-based chain whose stationary distribution is equivalent to the desired posterior.
- Delayed Rejection Adaptive Metropolis
- Here, we use a hierarchical DRAM-within-Metropolis algorithm to statistically infer all unknown quantities.
- Priors are uninformative, with starting values determined from frequentist maximum likelihood estimates.

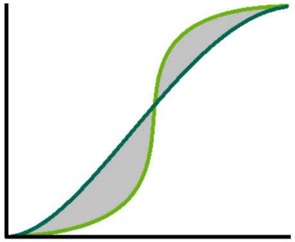
Validation: Uncertainty Propagation

- In most cases, a Monte-Carlo propagation is used to approximate the effect of parameter uncertainty on model results.
- Requires a large number of samples to accurately predict distribution of the quantity of interest (QoI), and can therefore be computationally intensive.
- Alternatively, Wilks' method can be used when comparison to safety or regulatory limits is required. This gives very little information about uncertainty or predictive capability.

Prediction: Validation Metrics

- Various methods to quantify the quality of code predictions in the presence of both measurement and prediction uncertainties.
- Frequentist and Bayesian hypothesis testing
  - Calculate a p-value or Bayes factor, which indicate confidence in null hypothesis.
- Reliability
  - The probability that the observed difference is within a small interval $P(-\epsilon \leq D \leq \epsilon)$.
  - Can be used to weight calibrated and "alternate" parameter distributions.
- Kolmogorov-Smirnov
  - Maximum vertical distance between two CDFs, $0 \leq KS \leq 1$
- Area Metric
  - Total area between two CDFs, positive
- Many others[1]



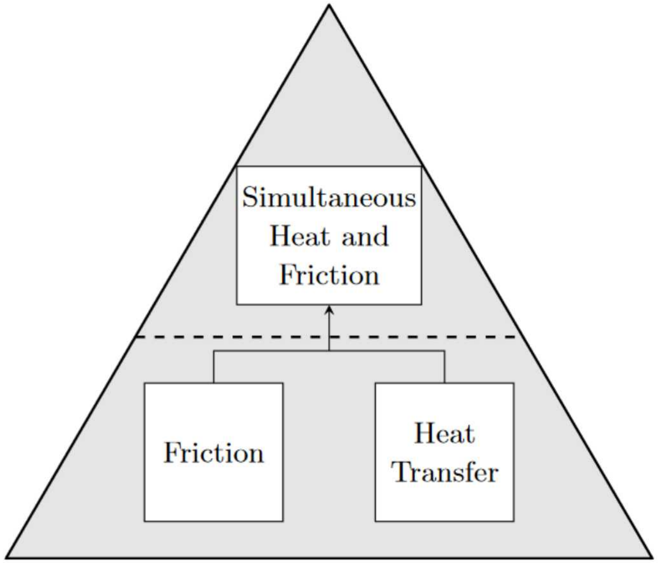


1. Maupin, K. A., and Swiler, L. P., 2017. Validation metrics for deterministic and probabilistic data. Tech. Rep. SAND2016-1421.

Demonstration

Case Study

- A simple problem is selected to demonstrate the framework.
- Friction and heat transfer in smooth tubes for turbulent flow.
- The calibration pyramid has three components:
  - Isothermal pressure drop experiments,
  - Heat transfer experiments where pressure drop is not measured, and
  - Simultaneous measurement of pressure drops and heat transfer.
- Here, we perform only the calibration exercise, since application to a "real world" problem would require more tiers in the pyramid.

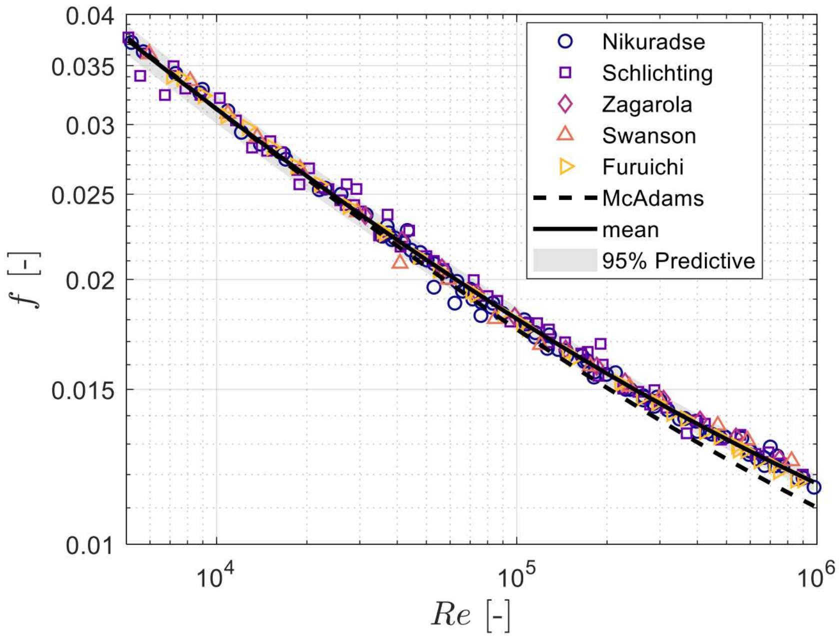


Friction

- McAdams relation: $f = 0.005 + 0.5Re^{-0.32}$
- Experiments of pressure drop measurements in horizontal smooth tubes.
- Here, the statistical model is determined via initial frequentist analysis (minimization of AIC and BIC): θ_1 is deterministic and $\theta_2 \sim N(\mu, \sigma^2)$.

$$f = \theta_1 + \theta_2 Re^{-0.32}$$

Year	Author	Pipe	Fluid
1932	Nikuradse[1]	Brass	Water
1982	Schlichting & Gersten[2]	Brass	Water
1998	Zagarola & Smits[3]	Aluminum	Air
2002	Swanson et al.[4]	Stainless steel	Gases, He
2015	Furuichi et al.[5]	Glass	Water



1. Nikuradse, J., 1966. Laws of turbulent flow in smooth pipes. Tech. Rep. TT 359, NACA. Translation of *Verein Deutscher Ingenieure-Forschungsheft*, 356(3), October 1932.
2. Schlichting, H., and Gersten, K., 1982. Boundary Layer Theory. Springer. Berlin, Germany.
3. Zagarola, M. V., and Smits, A. J., 1998. "Mean-flow scaling of turbulent pipe flow". *J Fluid Mech,* 373, pp. 33–79.
4. Swanson, C. J., et al., 2002. "Pipe flow measurements over a wide range of Reynolds numbers using liquid helium and various gases". *J Fluid Mech,* 461, pp. 51–60.
5. Furuichi, N., et al., 2015. "Friction factor and mean velocity profile for pipe flow at high Reynolds numbers". *Phys Fluids,* 27(9).

Heat Transfer

- Dittus-Boelter relation:

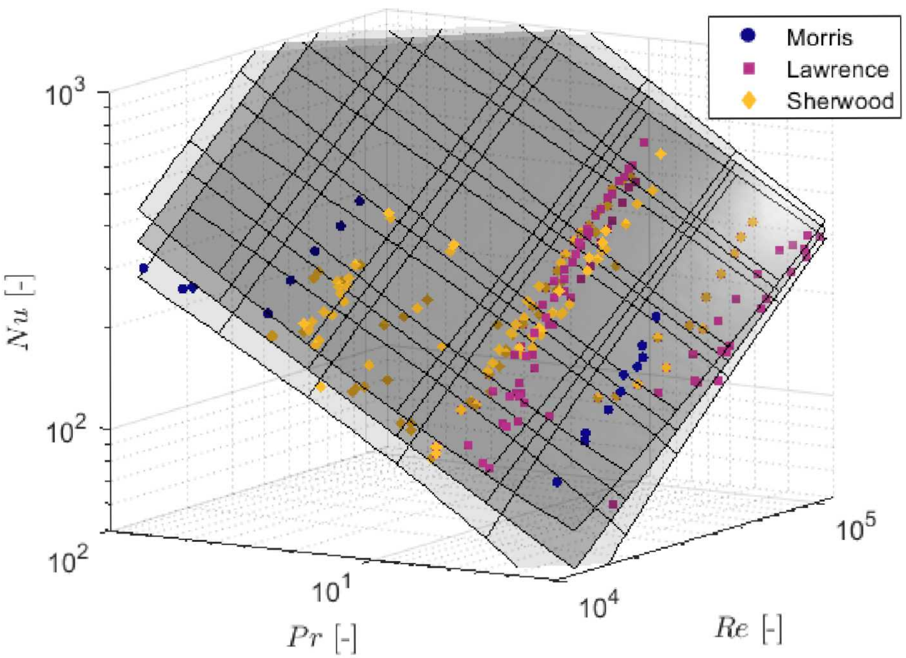
$$Nu = 0.023Re^{0.8}Pr^{0.4}$$

- Experiments of energy transfer to fluid flowing through hot smooth pipe.
- Statistical model: θ_3 is deterministic and $\theta_4 \sim N(\mu, \sigma^2)$.

$$Nu = \theta_3 Re^{0.8} Pr^{\theta_4}$$

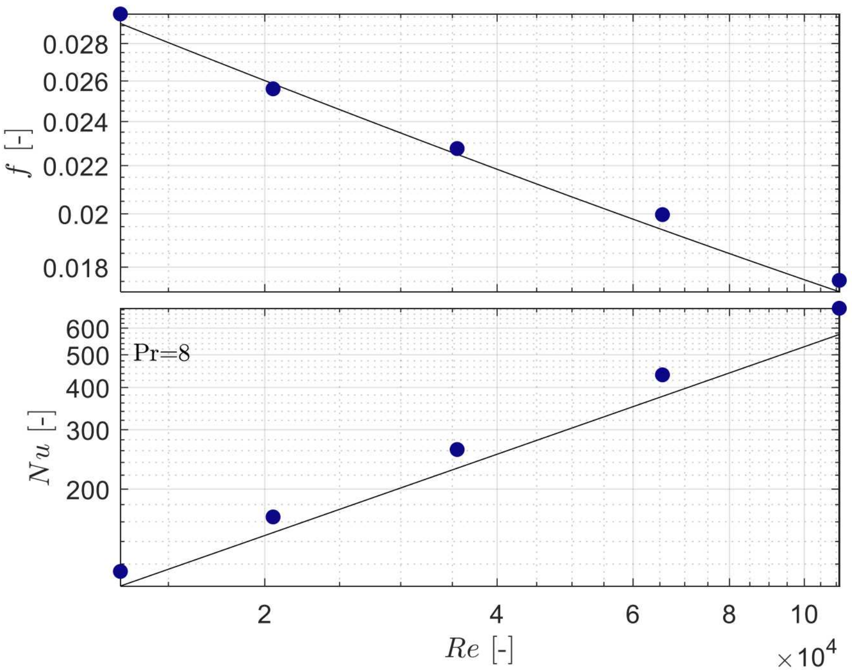
Year	Author	Pipe	Fluid
1928	Morris & Whitman[1]	Steel	Water & oil
1931	Lawrence & Sherwood[2]	Copper	Water
1932	Sherwood & Petrie[3]	Copper	Water

1. Morris, F. H., and Whitman, W. G., 1928. "Heat transfer for oils and water in pipes". *Ind Eng Chem*, 20(3), pp. 234–240.
2. Lawrence, A. E., and Sherwood, T. K., 1931. "Heat transmission to water flowing in pipes". *Ind Eng Chem*, 23(3), pp. 301–309.
3. Sherwood, T. K., and Petrie, J. M., 1932. "Heat transmission to liquids flowing in pipes". *Ind Eng Chem*, 24(7), pp. 736–745.



Simultaneous Friction & Heat Transfer

- We use the data of Allen & Eckert for simultaneous calibration of the friction factor and Nusselt number.
- Only five data points; sparsity of the data is typical of many engineering problems.
- The plot shows the data along with McAdams and Dittus-Boelter relations.
- Likelihood is formulated as sum of friction and Nusselt number likelihoods.
- Again, statistical models are formulated via initial frequentist analysis with minimization of information criteria.



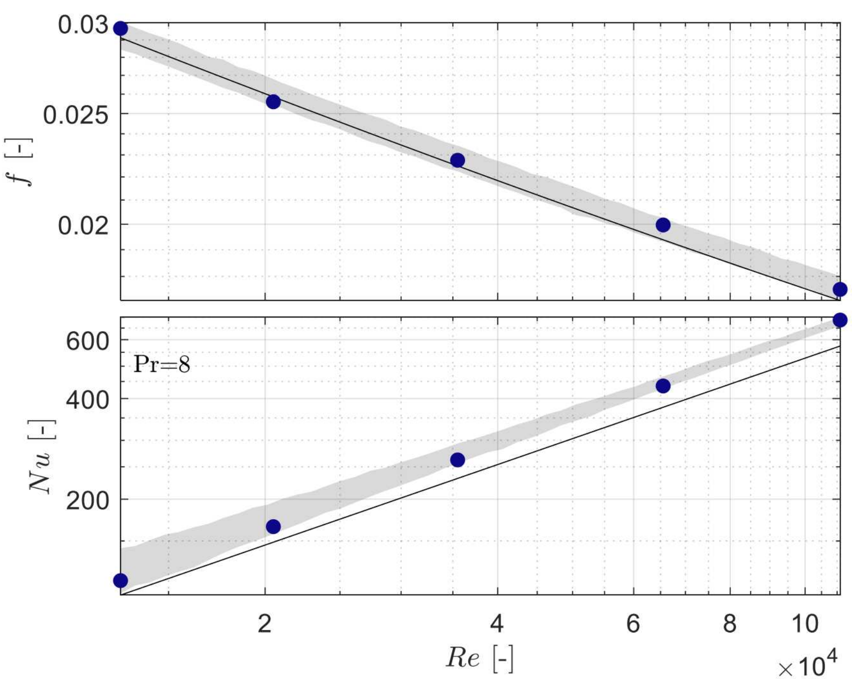
1. Allen, R. W., and Eckert, E. R. G., 1964. "Friction and heat-transfer measurements to turbulent pipe flow of water (Pr=7 and 8) at uniform wall heat flux". J. Heat Transfer, 86(3).

Simultaneous Friction & Heat Transfer

- First, we calibrate without using priors from separate effects data.
- Statistical model: Prandtl number is fixed, so Dittus-Boelter Prandtl exponent becomes unidentifiable. θ_1 and θ_3 are treated deterministically, $\theta_2 \sim N(\mu, \sigma)$.

$$f = \theta_1 + \theta_2 Re^{-0.32}$$
$$Nu = \theta_3 Re^{0.8} Pr^{0.4}$$

- Uncertainty in θ_4 is not treated, so error in Nusselt number grows at low Reynolds numbers.
- Heat transfer result is calibrated to only this data, so the bias compared to Dittus-Boelter relation is not represented.

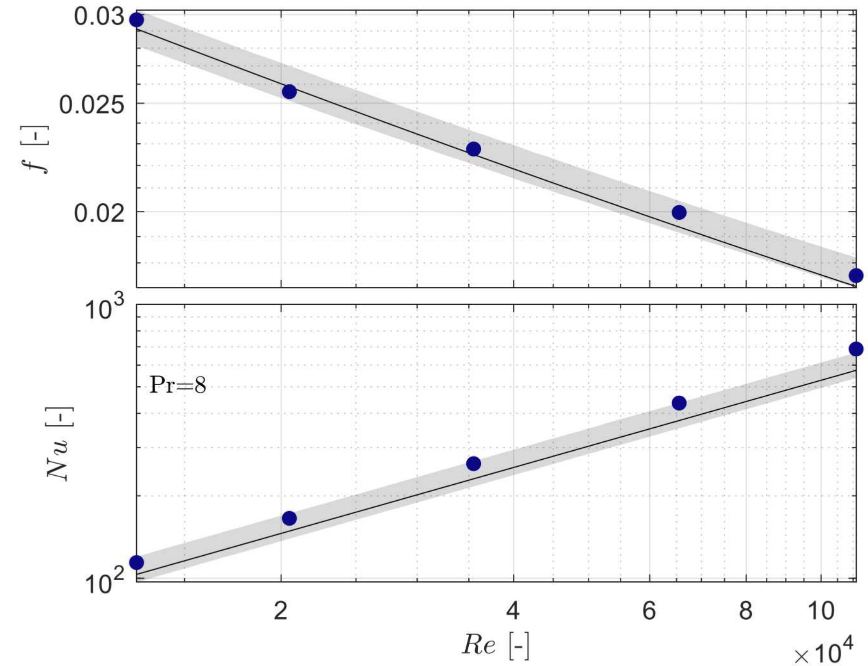


Simultaneous Friction & Heat Transfer

- Now, calibrate using separate effects results as priors.
- Statistical model: Dittus-Boelter Prandtl exponent becomes identifiable. θ_1 and θ_3 are treated deterministically, $(\theta_2, \theta_4) \sim N(\mu, \Sigma)$ with diagonal Σ.

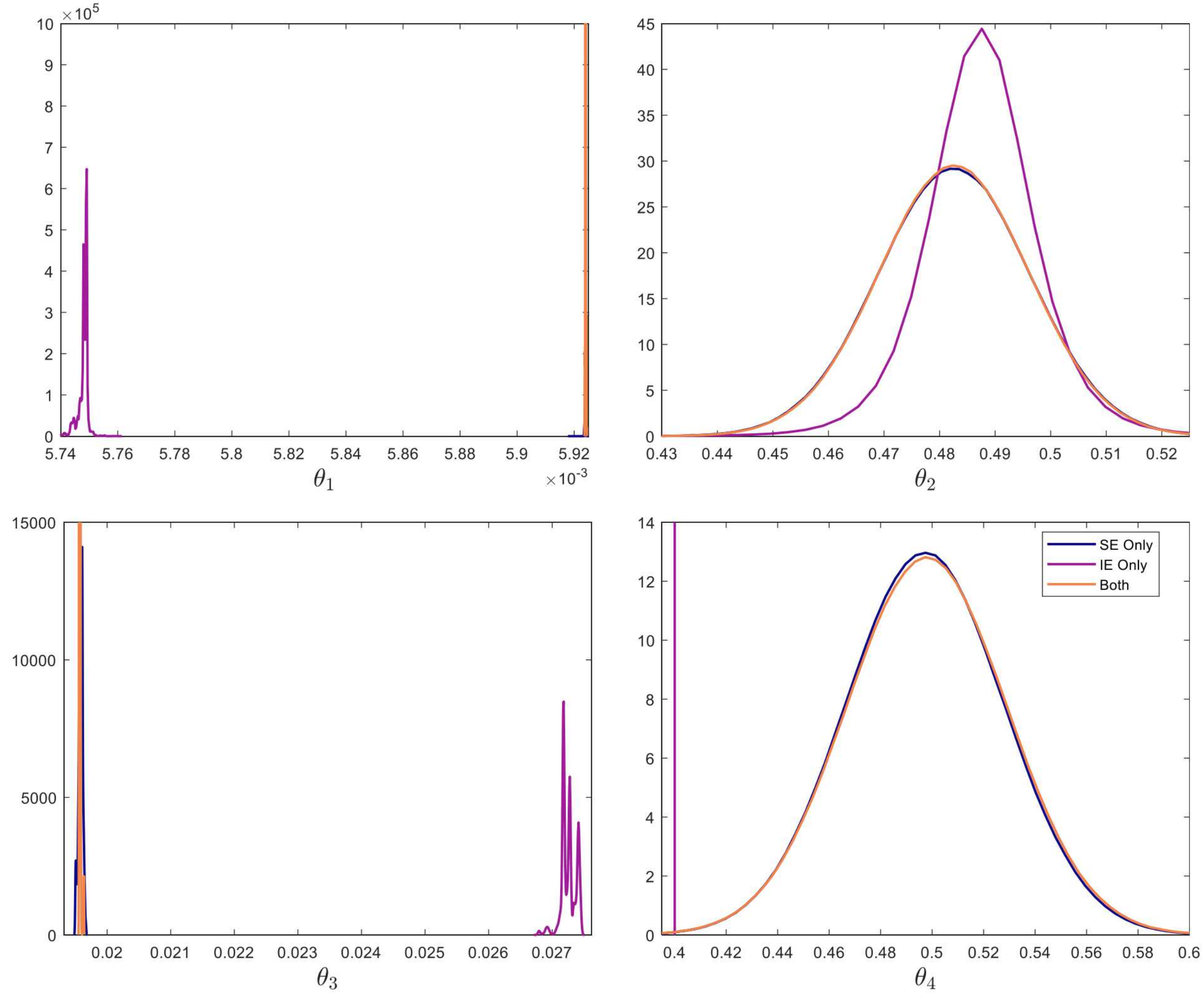
$$f = \theta_1 + \theta_2 Re^{-0.32}$$
$$Nu = \theta_3 Re^{0.8} Pr^{\theta_4}$$

- Correctly treating uncertainty in θ_4, so interval has the right shape.
- Heat transfer result correctly indicates that this data has a small positive bias.



Parameter Results

- Parameters are significantly different between SE and IE studies.
- Epistemic uncertainty in parameters θ_1 and θ_3 significantly reduced by addition of separate effects data.
- The parameter θ_4 was unidentifiable for the integral data; addition of separate effects data allows it to be estimated.



Conclusion

Discussion

- Given some data set and corresponding state variables:
  1. Bayesian analysis is used to find parameter estimates using a hierarchical structure with priors.
  2. The parameter estimates are propagated through the validation problem(s).
  3. Quality of the predication is quantified.
- Friction and heat transfer are empirical relations for the same physical process (boundary layers/turbulence), therefore the hyperparameters are not independent.
  - Chilton-Colburn analogy

$$\frac{Nu}{f} = 0.5RePr^{1/3}$$

  - In the future, this can be treated via a metropolis-within-DRAM hierarchical calibration, which allows accurate estimation of the hyperparameter covariance[1]

1. Schmidt, K. L., 2016. "Uncertainty quantification for mixed-effects models with applications in nuclear engineering." PhD thesis, North Carolina State University.

Conclusion

- Calibration to separate effects data can unidentifiability in the integral effects data due to model form, sparse data, or related physical processes.
- Separate effects data can also decrease epistemic uncertainty in models where integral tests have sparse data.
- It is important to not treat calibration/validation process or simulation model as "black boxes."
- This process may break down or result in large uncertainties for cases with low quality or quantity of data.
  - Large epistemic uncertainties indicate that data is too sparse.
  - Large aleatory uncertainty or noise indicate that the data is low quality.
  - Can be used to direct future experimental work.
- Simultaneously calibrating to multiple datasets is mathematically equivalent to successive calibrations with priors.

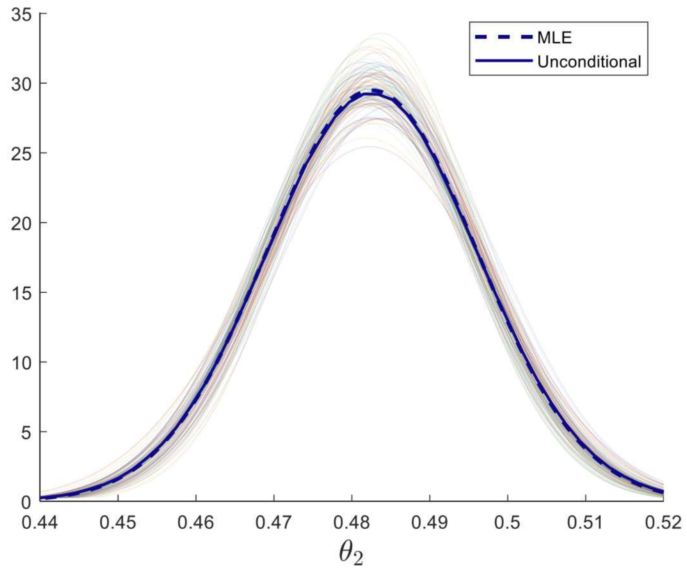
- Thanks to the following individuals for their assistance during the preparation of this work:
  - *Sandia National Labs*: Joshua G. Mullins, Laura P. Swiler
  - *Los Alamos National Lab*: Brian J. Williams
  - *North Carolina State University*: Paul R. Miles, Ralph Smith

Types of Distributions

- Maximum likelihood estimate (MLE): most accurate distribution, which excludes epistemic uncertainty.
- Unconditional distribution: includes both aleatory and epistemic uncertainty

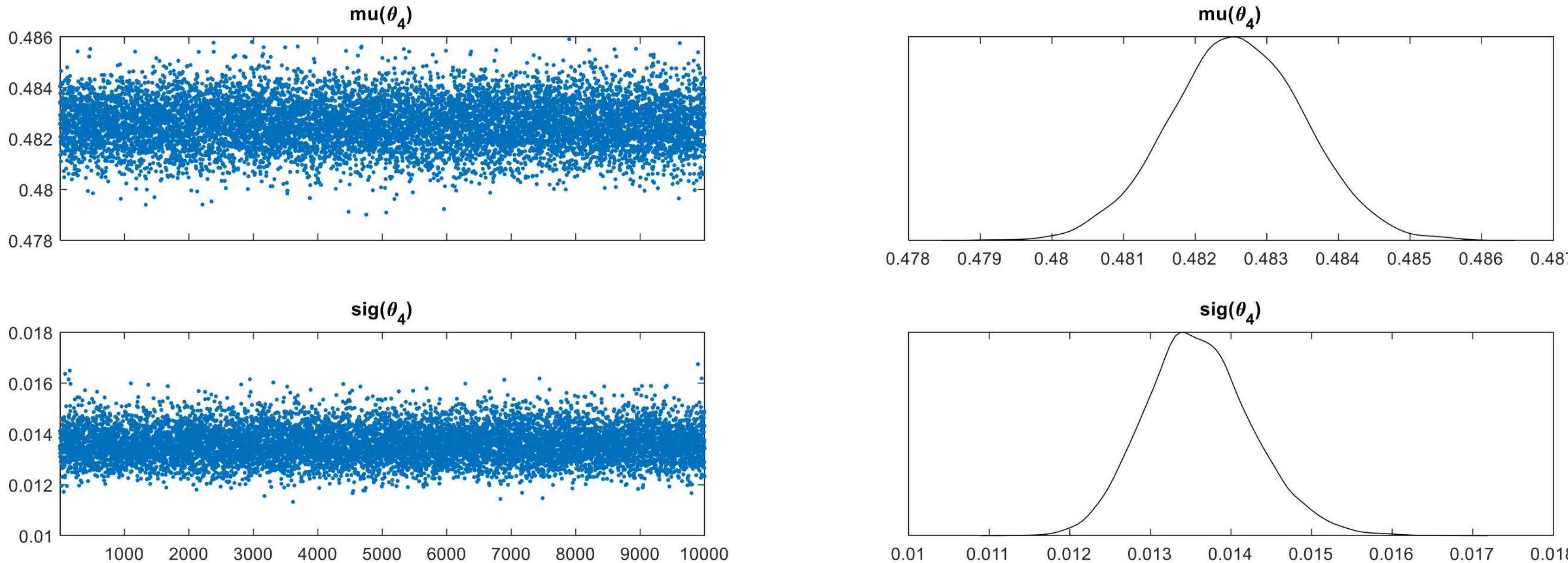
$$f_\Theta(\theta) = \int_D f_\Theta(\theta|\boldsymbol{P} = \boldsymbol{p}) f_P(\boldsymbol{p})\, d\boldsymbol{p}$$

- In this presentation, both aleatory and epistemic uncertainty are included in all distributions.



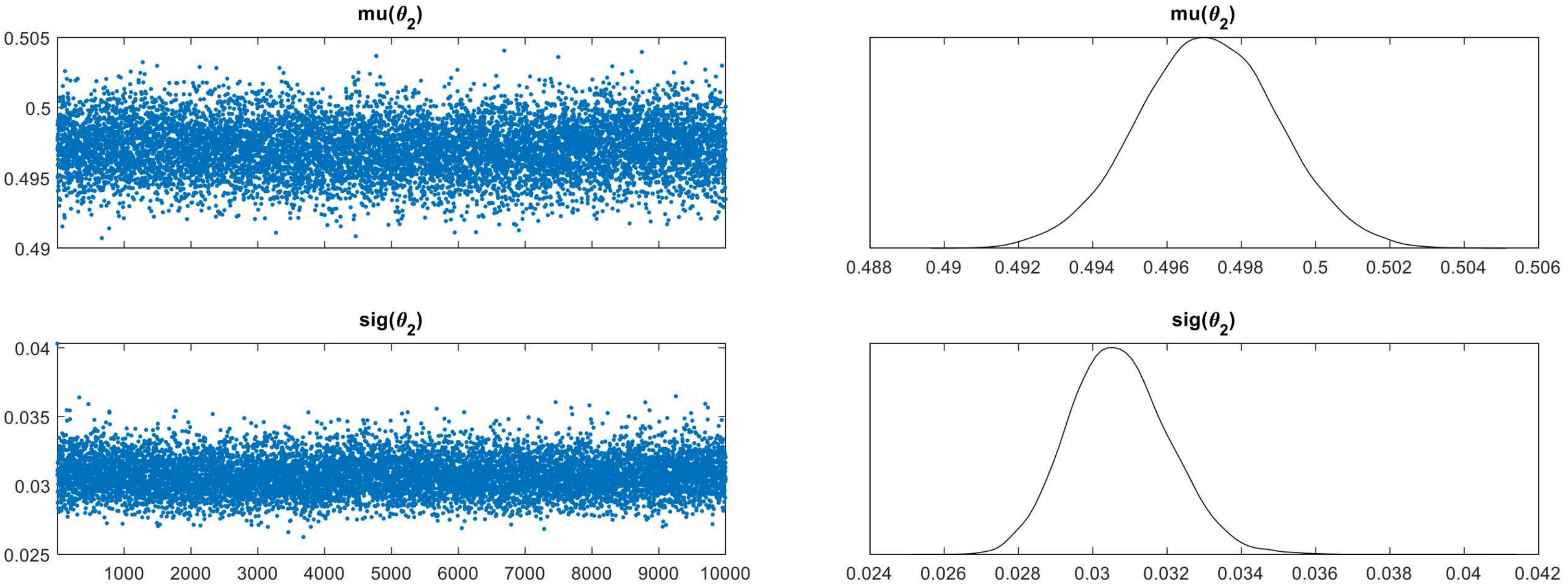
Friction Calibration

	mean	std	MC_err	tau	geweke
mu(\theta_4)	0.0059238	2.4415e-07	3.7964e-09	0.90063	1
sig(\theta_4)	0.48344	1.1076e-05	2.49e-06	706	0.9999



Heat Transfer Calibration

	mean	std	MC_err	tau	geweke
mu(\theta_2)	0.4971	0.0018767	4.5229e-05	1.1066	0.99963
sig(\theta_2)	0.030717	0.0013392	3.4161e-05	1.0807	0.99086



Simultaneous Calibration

	mean	std	MC_err	tau	geweke
mu(\theta_2)	0.482590	0.0009043	8.0967e-06	0.9714	0.99995
sig(\theta_2)	0.013545	0.0006455	6.865e-06	1.0015	0.99471
mu(\theta_4)	0.497870	0.0018685	1.8028e-05	1.0028	0.99994
sig(\theta_4)	0.031149	0.0013237	1.4554e-05	1.0371	0.99896