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Advances in Discrete-Direct Sparse-Sampling Approaches for Aleatory and Epistemic Uncertainties in Model Calibration and Inverse Problems

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Introduction to "Discrete Direct" (DD) approach for Model Calibration and Uncertainty Propagation problems involving Aleatory Variability

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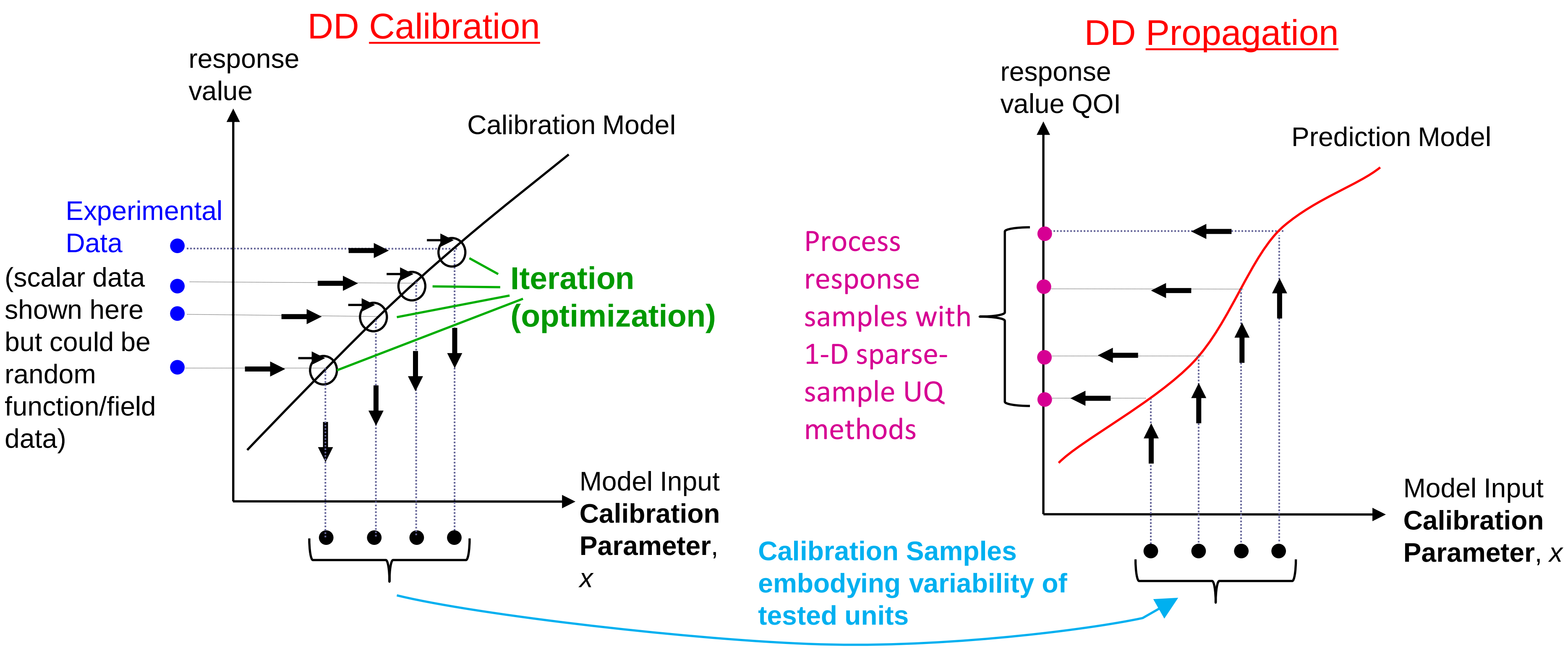
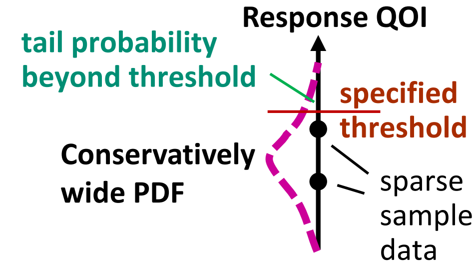


- **Propagate the discrete values of the calibration parameters**
- **Straightforwardly extends to problems with multiple calibration parameters**
- ***N* runs of model to propagate *N* param. values or sets from *N* calibration experiments**
- **Simple to update w/new experiments/data that may become available (w/out Bayes' rule & machinery)**

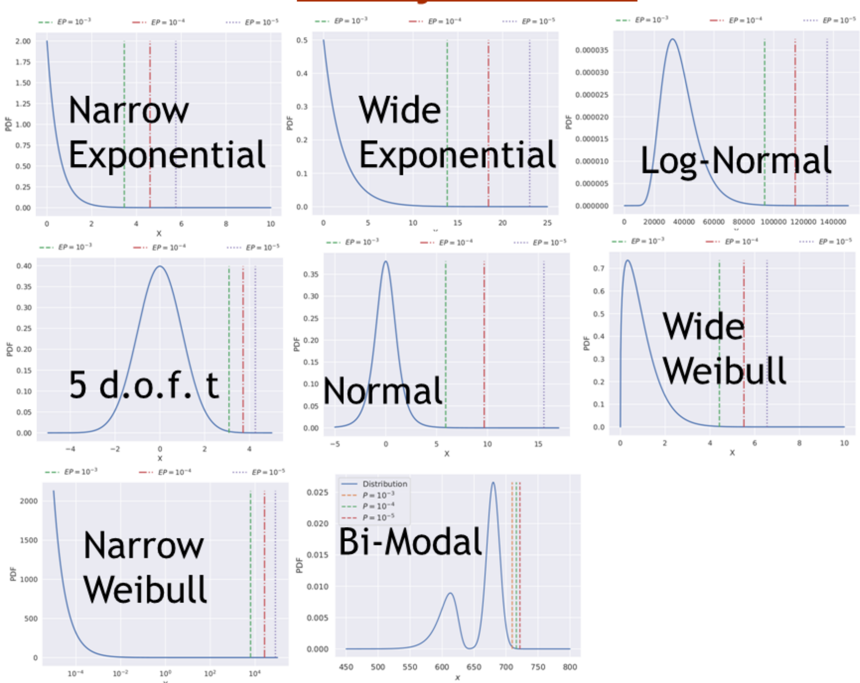
Testing and Optimization of Sparse-Sample 1-D UQ Methods for Conservative Tail-Probability Estimation

Objective: be conservative but not overly conservative (efficient)

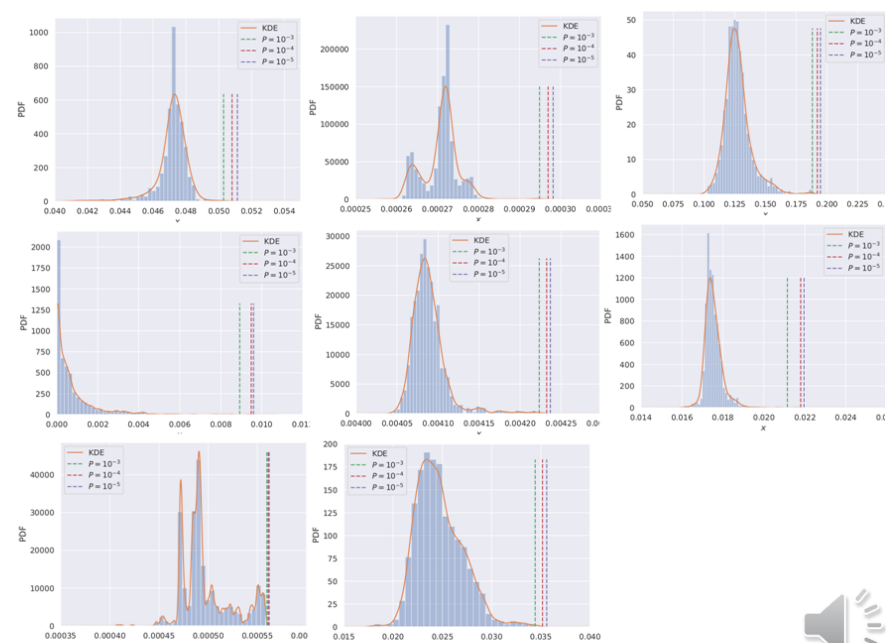


- Large numerical study with > 3e+08 performance tests
- ~20 established and newly developed methods (variants, hybrids)
- tail probability magnitudes 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}
- # samples N = 2, 3, 4,…,20
- 16 diverse distribution shapes below
- 10K random sampling trials for each combinations of the above factors studied

8 analytical PDFs



8 empirical PDFs



DD Simplicity, Cost, and Trustworthiness Advantages: maps Multi-D UQ ➡ 1-D UQ

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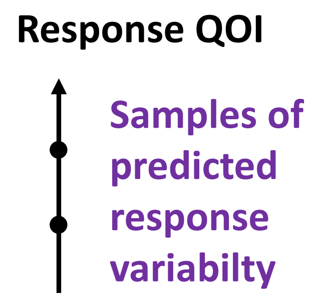
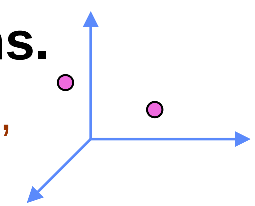
- **Example**:
  - a model with 3 calibration parameters
  - N=2 replicate experiments



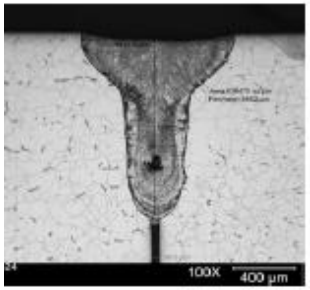
- **DD: 2 calibrations ➔ 2 parameter sets ➔ 2 runs of prediction model ➔ 2 values of response**
  - get a 1-D UQ problem with 2 samples of response
  - Get reliable bounding estimates on response statistics

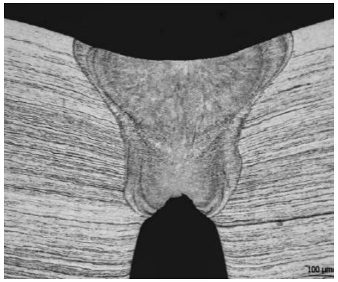
- **Distribution-based cal. parameter uncertainty representation & propagation approaches like Bayesian would need to infer a 3-D Joint PDF of param. variability from the 2 calibration parameter sets (data points) in the 3-D space of the calibration params.**
  - get a **highly questionable** JPDF and predicted PDF of response, uncertainty would be difficult and expensive to reliably estimate
  - JPDF propagation requires high expense or a surrogate model (added complexity, uncertainty, and more runs of the prediction model than DD)

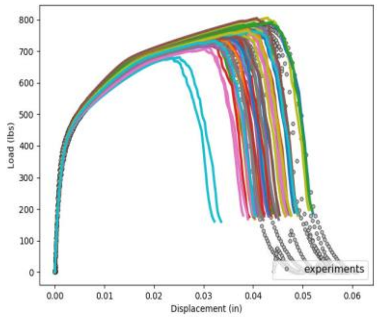


Confirmation of DD Calibration-Propagation-UQ method on Weld Depth and Strength Variability test problem

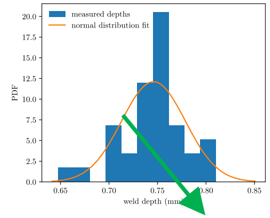
Pose 1000 weld-model calibration parameter sets that yield representative curve shapes and a population that envelopes 7 actual tension tests and stress-strain curves



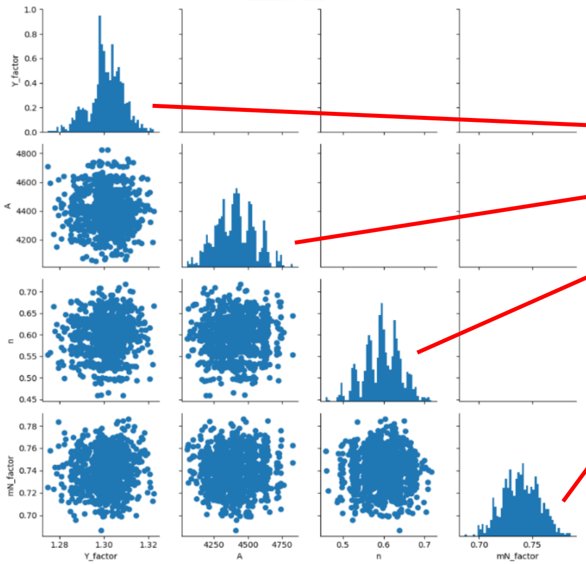




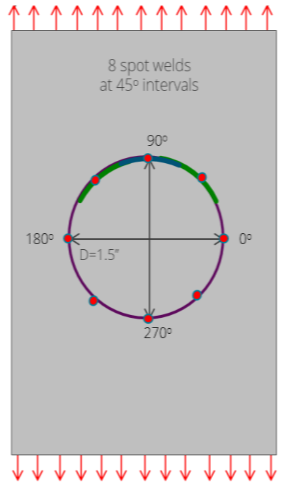
1000 random samples from Normal distribution fit to 34 weld-depth (D) measurements



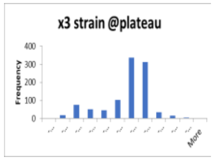
simulate Circular Laser Weld Test using input parameter sets

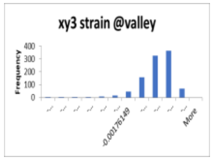


input parameter sets (Y, A, n, ϕ, D)$_j$ j = 1, 1000



- 1000 values for each output response quantity of interest (QOI)
  - example QOI histograms

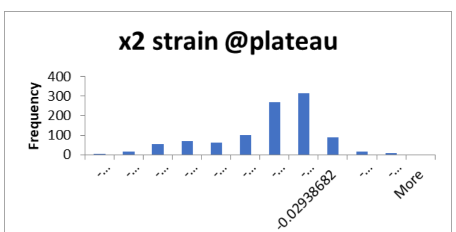


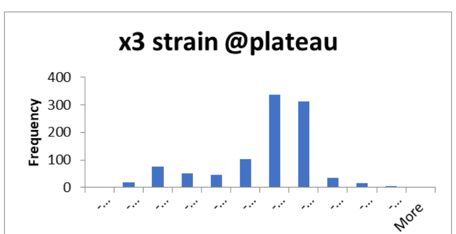


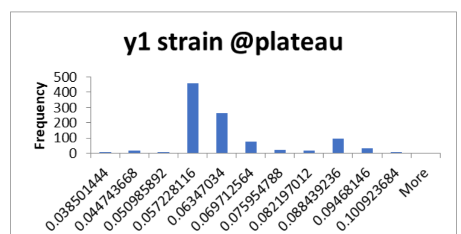
- 40 QOIs/histograms

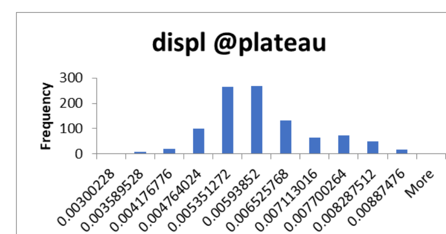
Performance on QOI tail-probability estimation

- **Conduct 250 random trials of the DD calibration-propagation-UQ method**
  - Each trial
    - N=4 material tests (replicate tests) for calibrating N=4 material plasticity and damage parameter sets
    - Combine the N=4 calibration parameter sets and N=4 weld-depth measurement samples and propagate through Circular Laser Weld structural model 🠲 4 samples of each QOI 🠲 **use statistically biased 1D UQ tail-probability estimation methods** for conservative estimation of **0.005 left and right tail probabilities of the 40 QOIs**
  - **40 challenging response QOI distributions (80 tails)**
    - most are highly Non-Normal — skewed, long-tailed, and/or multi-modal, some with bumps far out in the tails (examples below)









DD method High Success/Reliability rates of Conservative Tail-Probability Estimation for 80 Diverse Tails (Truth tail probabilities = 0.005)

- **Postprocess the 4 response samples per QOI (per trial) with the following conservatively biased 1D UQ tail-probability estimation methods**

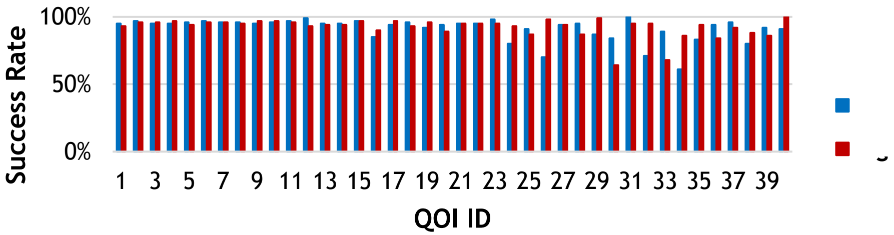
Tolerance Interval Equivalent-Normal method
(very simple, easy)

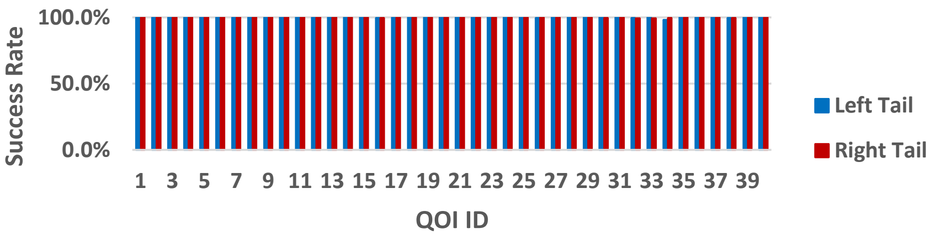
- **94% success rate of conservative tail-probability estimation over the 20,000 trials (80 diverse tails x 250 trials per tail)**
- average conservatism (mean bias) of estimates = 1.5 orders of magnitude

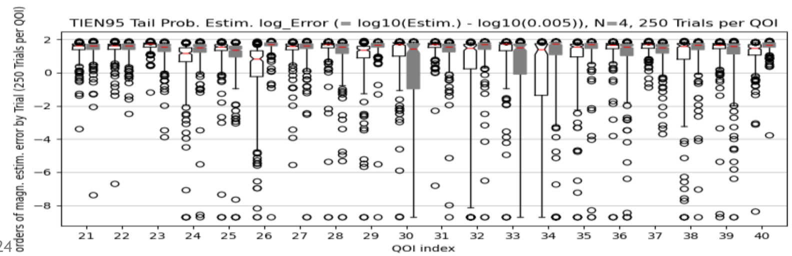
Super-Distribution Complete Jackknifing
(somewhat more complex)

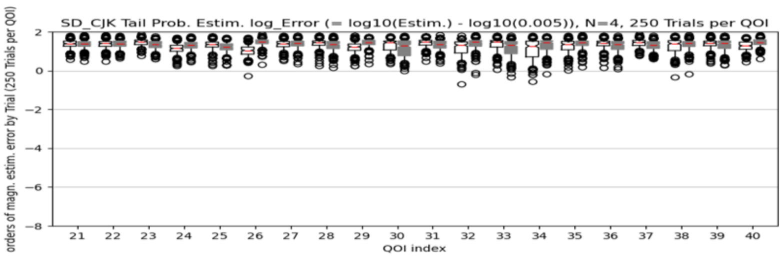
- **99.9% success rate of conservative tail-probability estimation over the 20,000 trials**
- average conservatism (mean bias) = 1.3 orders of magnitude

250 random trials for each of 80 diverse tails









DD Methodology applied to Strain-Rate Dependent Plasticity Model calibrated to Sparse Random Field Data

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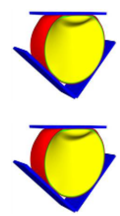
I.

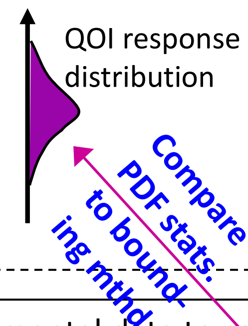
JC model parameter variations below emulate physical material variability → Evaluate component model responses (output QOIs of Can-Crush problem) → Form populations/distributions of QOI response and selected statistics

$(A,B,C,n)_1$

⋮

$(A,B,C,n)_{100}$





potential desired statistics

- *percentiles*
- *tail probabilities*

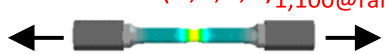
II

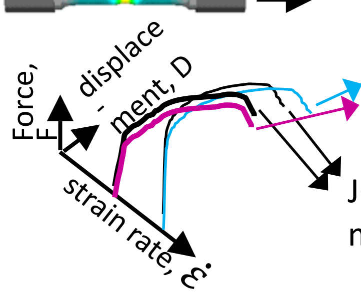
Experimental Design for Calibration Data: Propose material tension tests at various strain rates → Use experimental data to calibrate JC model to predict component-level responses/QOIs that reflect effects of material variability

Example - 4 uniaxial tension tests

- **2 strain rates X 2 tests each**

Use JC with $(A,B,C,n)_{1,100@random}$

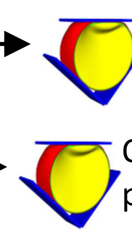


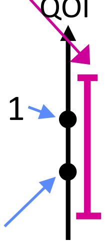


One possible combination…

JC calibration to mtl. curves Set 1 → QOI prediction 1

JC calibration to mtl. curves Set 2 → QOI prediction 2





Confirmation on Can Crush test problem:

—DD performance for bounding the 5-95 percentile ranges of 16 mildly to highly non-Normal PDFs of response QOIs

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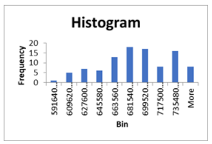
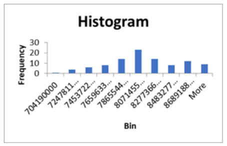
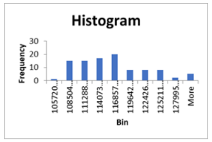


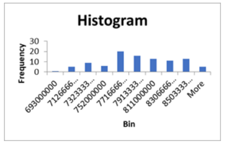
Max Von Mises stress, Weld I 0.25 time fraction



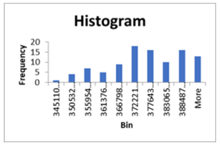
Max Von Mises stress, Weld I 0.5 time fraction



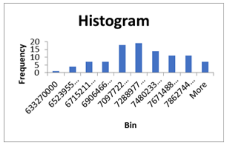
Von Mises stress, Weld 0.25 time fraction



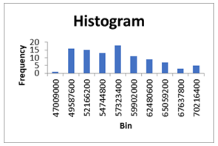
Von Mises stress, Weld 0.5 time fraction



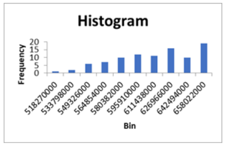
Von Mises stress, Lid Buckle 0.25 time fraction



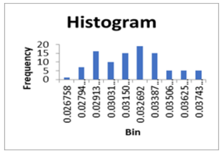
Von Mises stress, Lid Buckle 0.5 time fraction



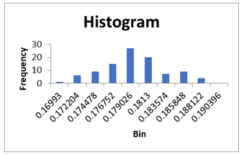
Von Mises stress, Can Top 0.25 time fraction



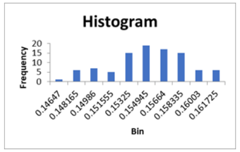
Von Mises stress, Can Top 0.5 time fraction



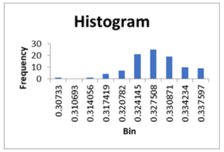
Max EQPS, Weld I 0.25 time fraction



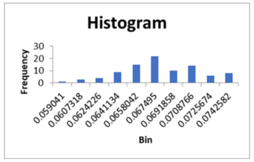
Max EQPS, Weld I 0.5 time fraction



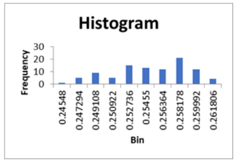
EQPS, Weld 0.5 time fraction



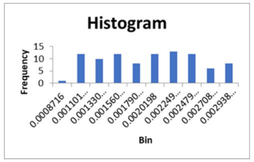
EQPS, Weld 0.75 time fraction



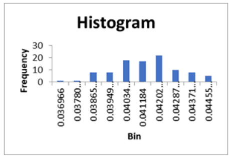
EQPS, Lid Buckle 0.5 time fraction



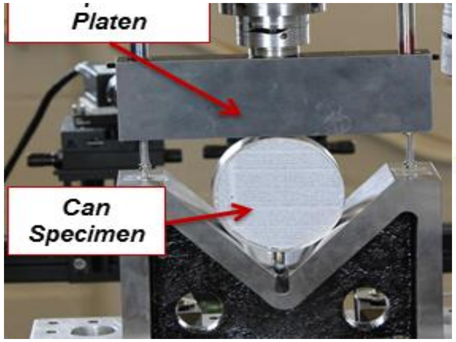
EQPS, Lid Buckle 0.75 time fraction

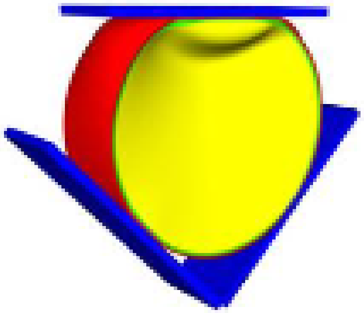


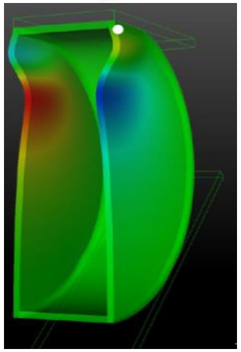
EQPS, Can Top 0.5 time fraction



EQPS, Can Top 0.75 time fraction







- 95/90 Tolerance Intervals used (based on 2 samples of QOI response from DD calibration and propagation of 2 cal. param. sets per trial)
- 20 random trials
- **92% success rate** over the 320 trials (= 16 QOIs x 20 trials/QOI)

DD calibration-propagation-UQ applied to Bolt Failure Modeling

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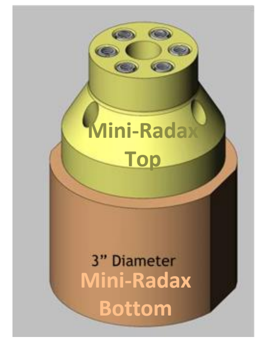
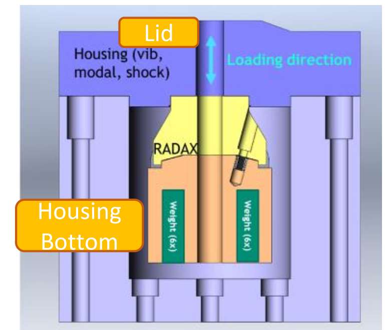
Uncertainty Quantification for Component Modeling Using the Discrete-Direct Approach

John P. Mersch
Paul R. Miles
Deborah M. Fowler
Christopher M. Laursen
Brian Fuchs





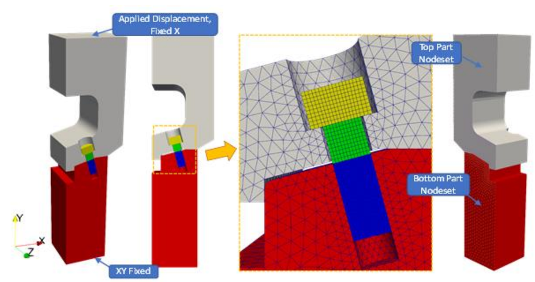
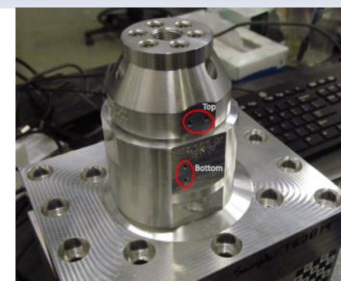


Figure 1. Single-Coupon Analysis Model



Other work in progress by Mersch et al:

"Discrete-Direct Uncertainty Quantification for Prediction of Fastener Failure in Sandia Mechanics Challenge"
—challenge problem developed by Sandia experimentalist Sharlotte Kramer

Accounting for IC/BC Control Variability and Non-Traveling Uncertainties in the Calibration Experiments and Computations (use model val. tech.)

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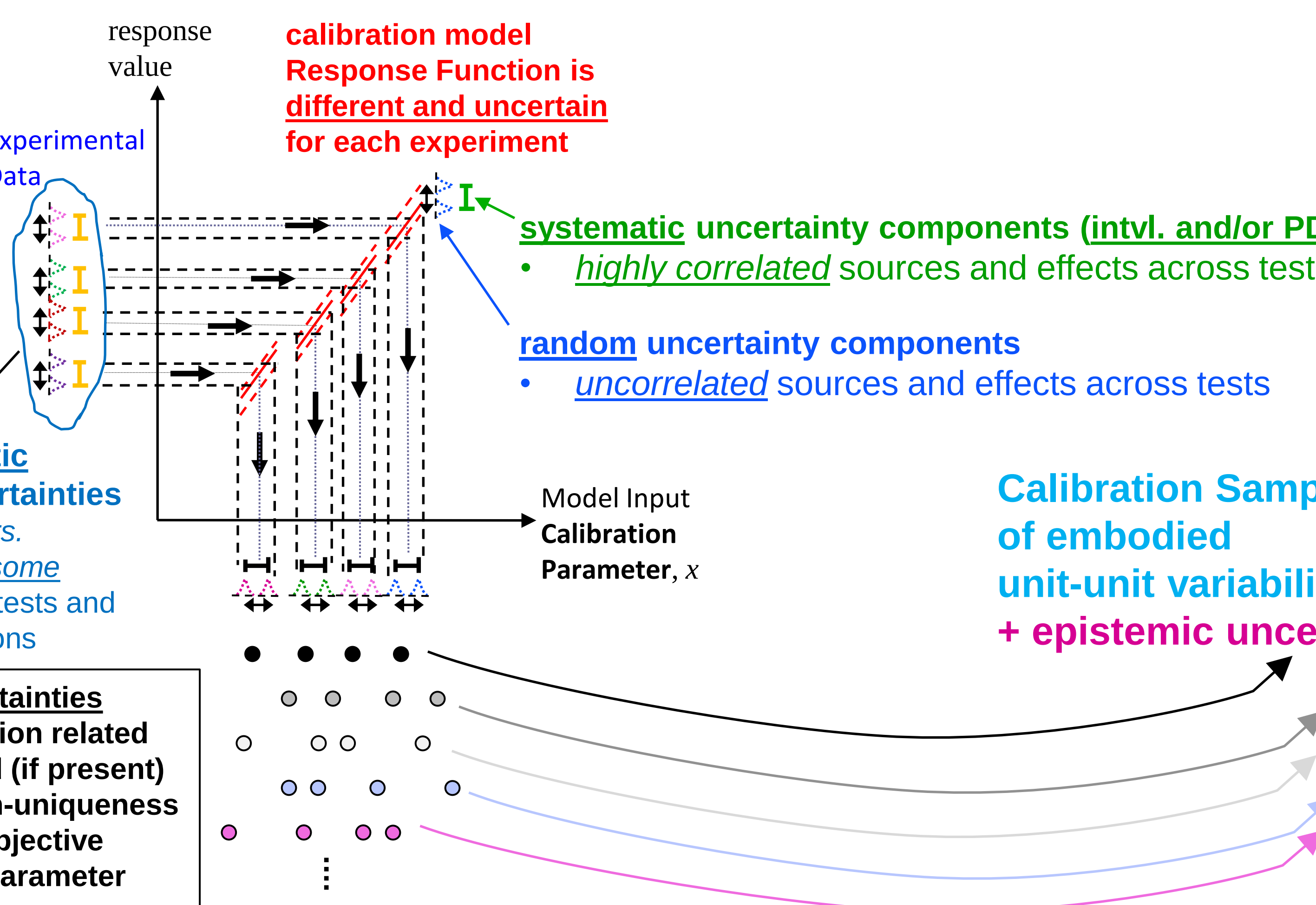
DD Approach for problems with both Aleatory AND Epistemic uncertainties



systematic uncertainty components (intvl. and/or PDF)
- *highly correlated* sources and effects across tests

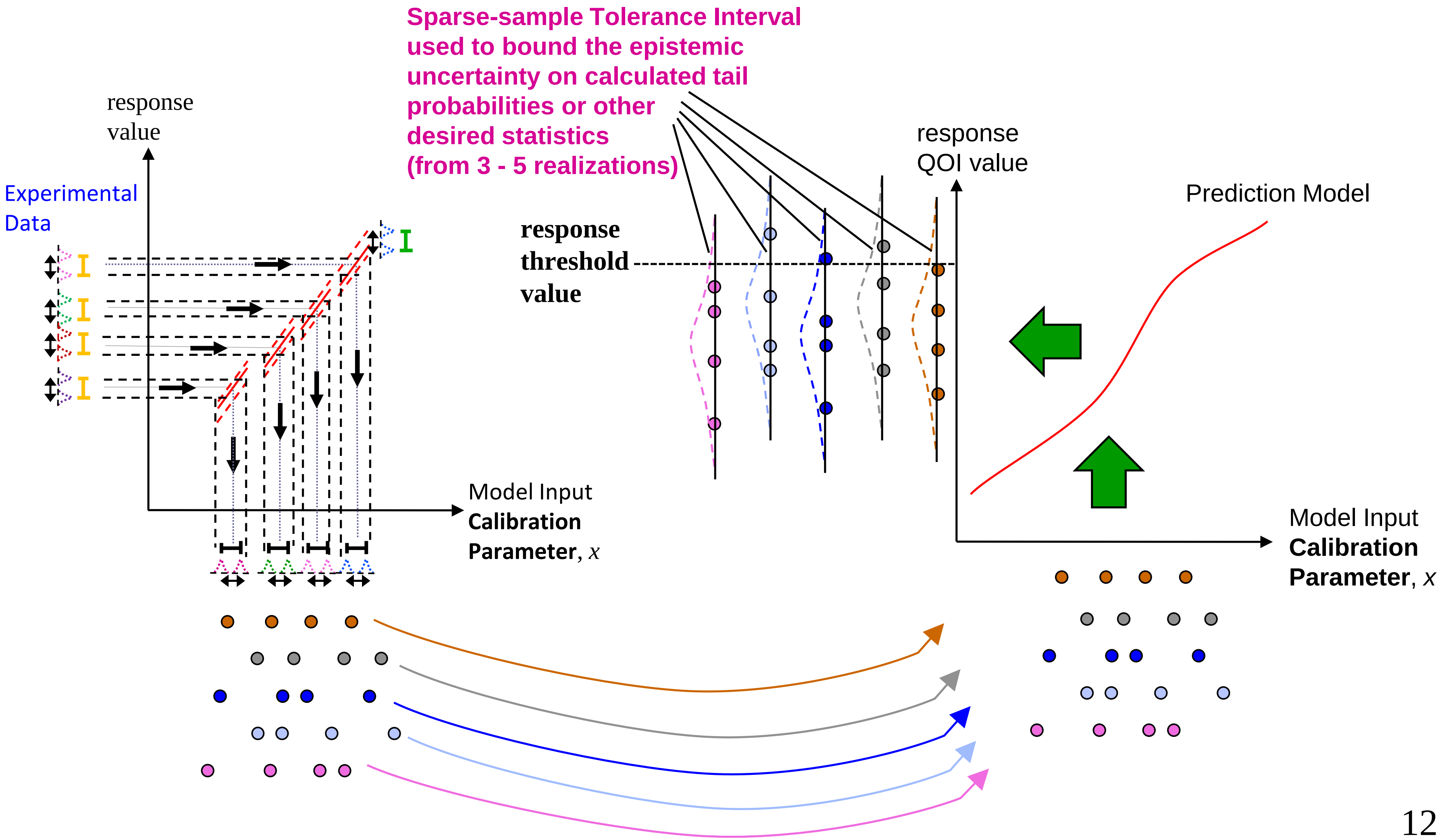
random uncertainty components
- *uncorrelated* sources and effects across tests

random & systematic measurement uncertainties
- *some errors/uncers. independent and some correlated* across tests and therefore calibrations

Calibration Samples of embodied unit-unit variability + epistemic uncertainty

Computational uncertainties
- **Model discretization related**
- **Surrogate related (if present)**
- **Opt. solution non-uniqueness due to noise in objective function and/or parameter non-identifiability**

DD Propagation of Calibration Parameter Sets reflecting Aleatory Variability and Epistemic Uncertainty, with UQ Processing of Response Samples



DD Calibration-Propagation-UQ with Epistemic Uncer. Only

(case of 1 calibration test—no replicate tests for elucidating unit-to-unit variability of modeled systems—Bayesian calibration becomes more competitive for epistemic-only cases)

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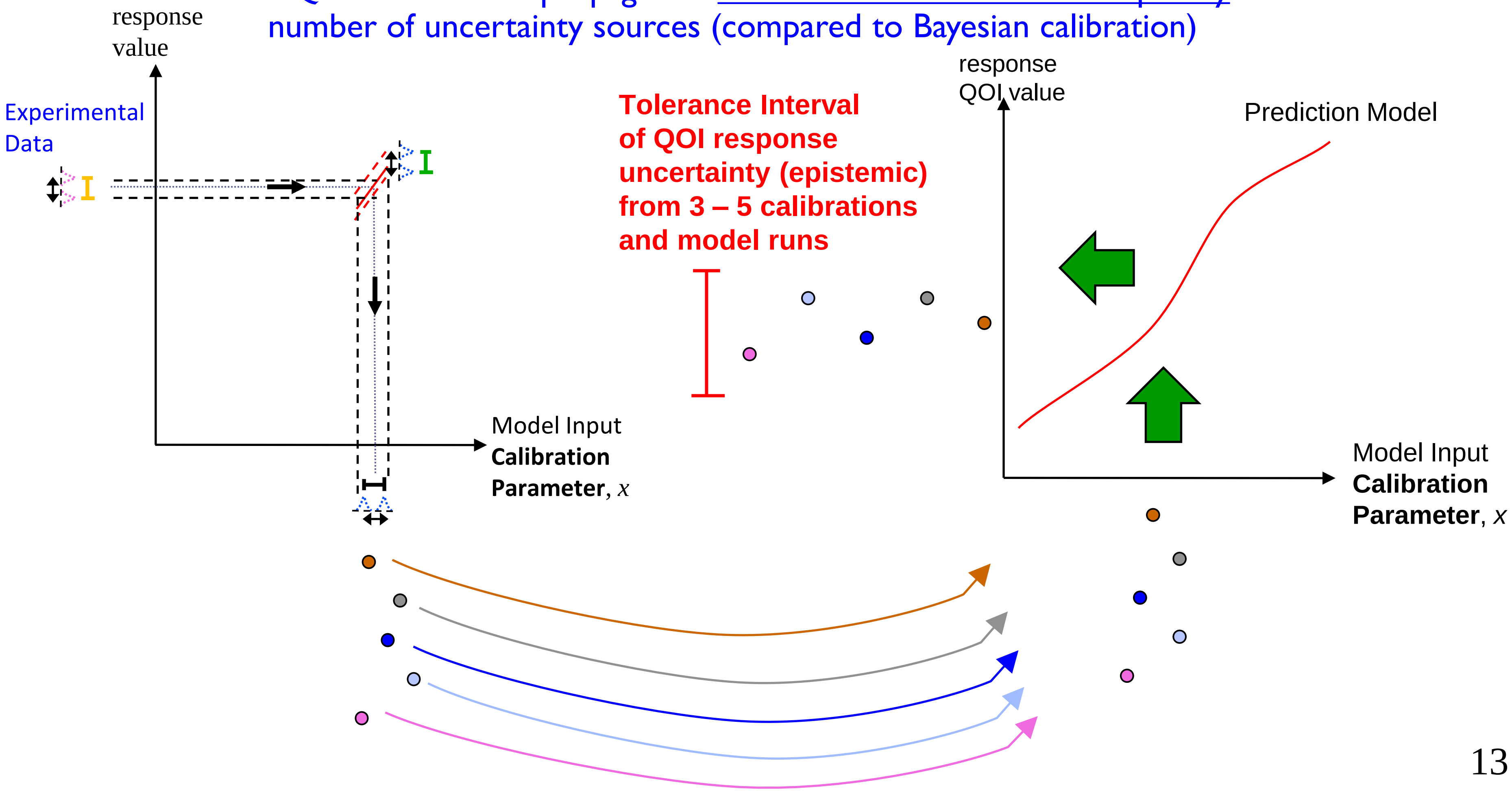
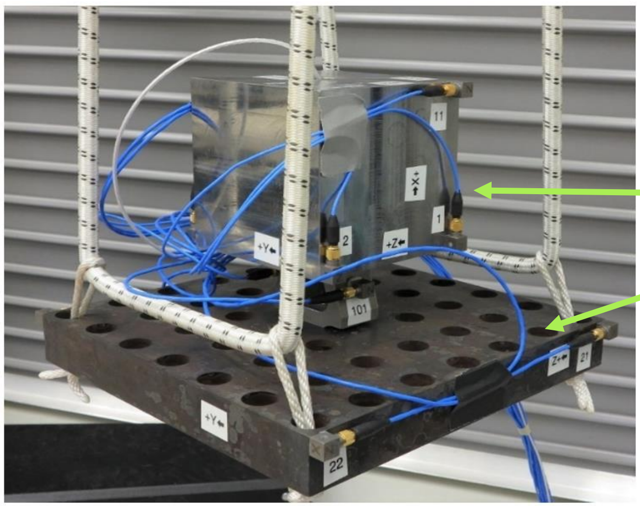
- Straightforward and Transparent treatment of various types and sources of epistemic uncertainties in experiment inputs and outputs (ICs, BCs, auxiliary/other)
- UQ treatment and propagation does not scale in cost or complexity with the number of uncertainty sources (compared to Bayesian calibration)



DD Application to Bolted-Joint Parameter Inversion in structural dynamics application

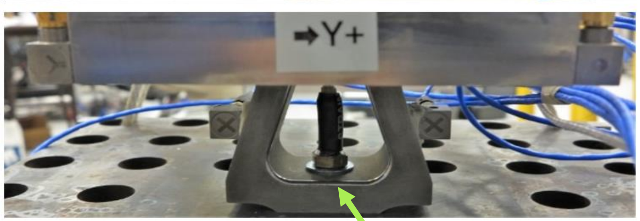
- **Calibrate 6 stiffness parameters of joint2g model**

Kettlebell Assembly test setup

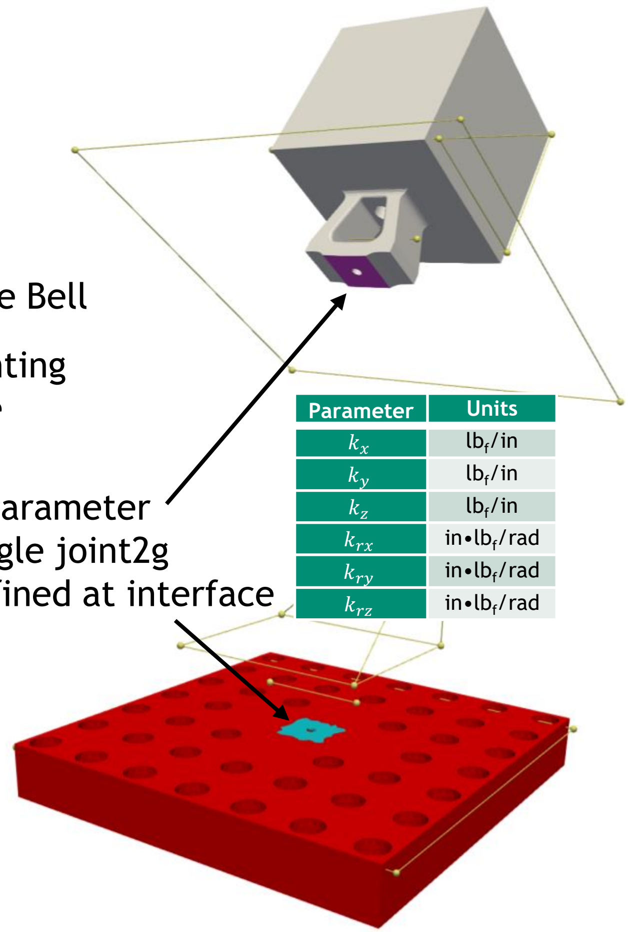


Kettle Bell

Mounting Plate



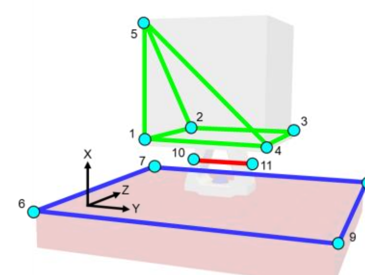
Strainsert Bolted Joint



6-parameter Single joint2g defined at interface

Parameter	Units
k_x	lb_f/in
k_y	lb_f/in
k_z	lb_f/in
k_{rx}	in•lb_f/rad
k_{ry}	in•lb_f/rad
k_{rz}	in•lb_f/rad

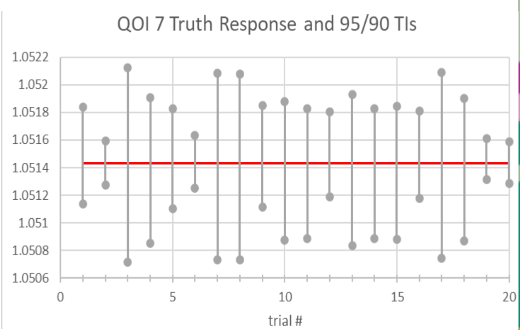
11 Accelerometer sensors



DD "Cross Prediction" approach for Epistemic Uncertainty in the 6 calibration parameters due to Limited Sensors

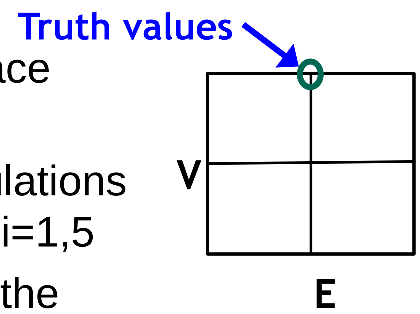
- **Test Problem Setup:**
  - Take the solution for the 6 parameters of the Kettle-Bell problem given the actual experimental conditions and sensor information
  - The 6 parameter values become the exact-known values in a test problem where they are prescribed to the joint and then synthetic BCs close to those in the experiment are prescribed for the shaker plate and outputs at the 11 sensor locations are obtained.
  - Using the limited (11) sensors data set in an inversion yields slightly different values for the 6 parameters than if a fuller set of sensors is used
- **Leave-1-out "Cross Prediction" approach to account for limited sensors**
  - Pick 5 different sensors at random, eliminate each (one at a time) and solve the parameter inversion problem based on information from the remaining 10 sensors
  - The parameter values in the five sets yield 95/90 TIs that capture the true values of the parameters
  - When the five param. sets are propagated through 7 posed next-level output QOI functions (at right), the 7 QOI 95/90 TIs capture the 7 QOI truth values
  - Same in 19 other trials — 100% success

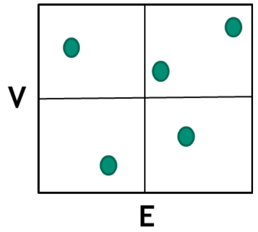
7 QOI test functions of the six calibration parameters
QOI 1 = KX + KY + KZ + KRX + KRY + KRZ
QOI 2 = KX − KY + KZ − KRX + KRY − KRZ
QOI 3 = KX + KY + KZ − (KRX + KRY + KRZ)
QOI 4 = √KX + √KY + √KZ + √KRX + √KRY + √KRZ
QOI 5 = √KX − √KY + √KZ − √KRX + √KRY − √KRZ
QOI 6 = √KX + √KY + √KZ − (√KRX + √KRY + √KRZ)
QOI 7 = (KX*KY*KRY)/(KZ*KRX*KRZ)



DD approach for Uncertainty in the 6 calibration parameters due to "Auxiliary" Epistemic Uncertainties in the experiments

- **Test Problem featuring uncertain values of Kettlebell material properties**
  - Let **truth values** of Young's Modulus (E) and Poisson's Ratio (V) lie on an edge of a prescribed E-V UQ space (10% and 17% uncertainties for E and V respectively)
  - Sparsely sample the E-V UQ space and perform inverse calculations for the 6 calibration parameters given each sample pair $(E,V)_i$ i=1,5
  - The 5 inversions have variously good objective function fits to the calibration data (from the 11 sensors) that correlates with how close the $(E,V)_i$ sample points are to the truth point $(E,V)_{Truth}$
  - Weight the parameter sets by log(1/objective_function_value)
  - Propagate the 5 parameter sets to the 7 QOI functionals and form 95/90 TIs from the weighted means and standard deviations of the 5 sample values of each QOI_k k=1,7
  - See if QOI_k 95/90 TIs capture $(QOI_k)_{Truth}$





- **Results of Random Trials**
  - 8 trials of random point sets $(E,V)_i$ i=1,5
  - For all 8 trials, for all k the QOI_k 95/90 TIs captured $(QOI_k)_{Truth}$
  - 100% success in the 8x7 = 56 tests
  - 100% success as well in 56 tests using only 3 uncertainty realizations $(E,V)_i$ i=1,3

Closing Remarks

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- **The DD approach is versatile and relatively simple, economical, and effective**
  - especially for physical systems involving significant unit-to-unit aleatory variability and models being calibrated for them