Design of Experiments (DOEs)

SmartUQ

- Features collection of highly efficient DOEs including Latin Hypercube Designs (LHDs)
- Sobol sequence

Unique Tools

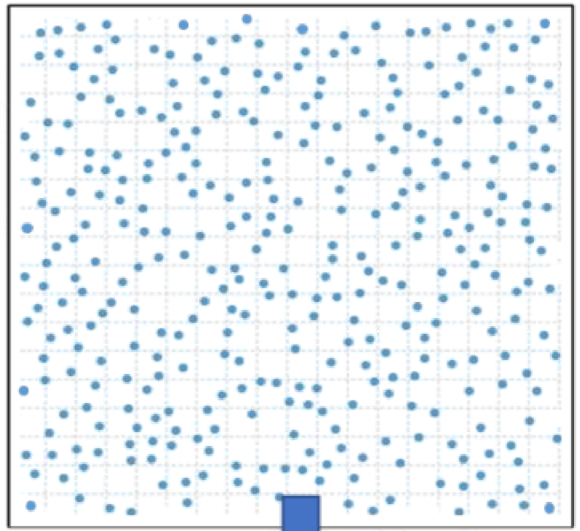
- Constrained DOEs: Uniformly distributes samples for highly constrained input spaces.
- Sliced LHDs
- Nested LHDs
- DOEs for Model Calibration

OpenTURNS

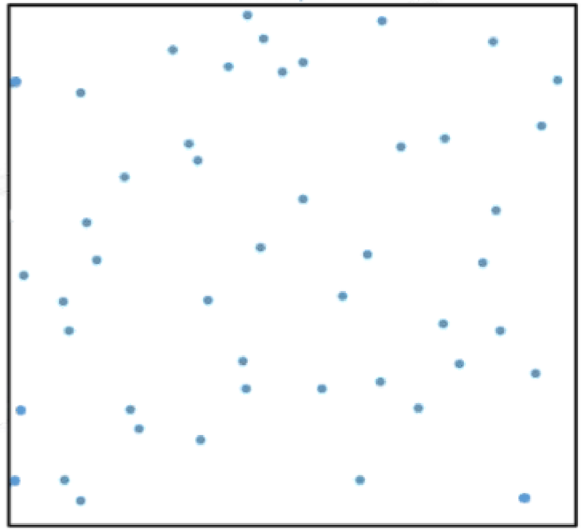
- Latin Hypercube Designs (LHDs)
- Quasi Monte Carlo sequences, e.g. Sobol sequence.
- Gauss Product and Composite
  - Similar to SmartUQ Full and Sparse Grid designs
  - Typically used for polynomial chaos expansion.
- Larger selection of traditional deterministic DOEs

Unique to SmartUQ: Reduce Large Data Set by Intelligent Subsampling

- **Subsampling** selects points to mimic a space-filling DOE:
  - Reduces potential for bias in the subsampled data.
  - Minimizes the number of points required for accurate predictive model creation.
  - Remaining data points may be used to validate the model.
- **Engineering Application:**
  - Reduce predictive model computations by creating a subsample from a previously collected high frequency sensor data set.



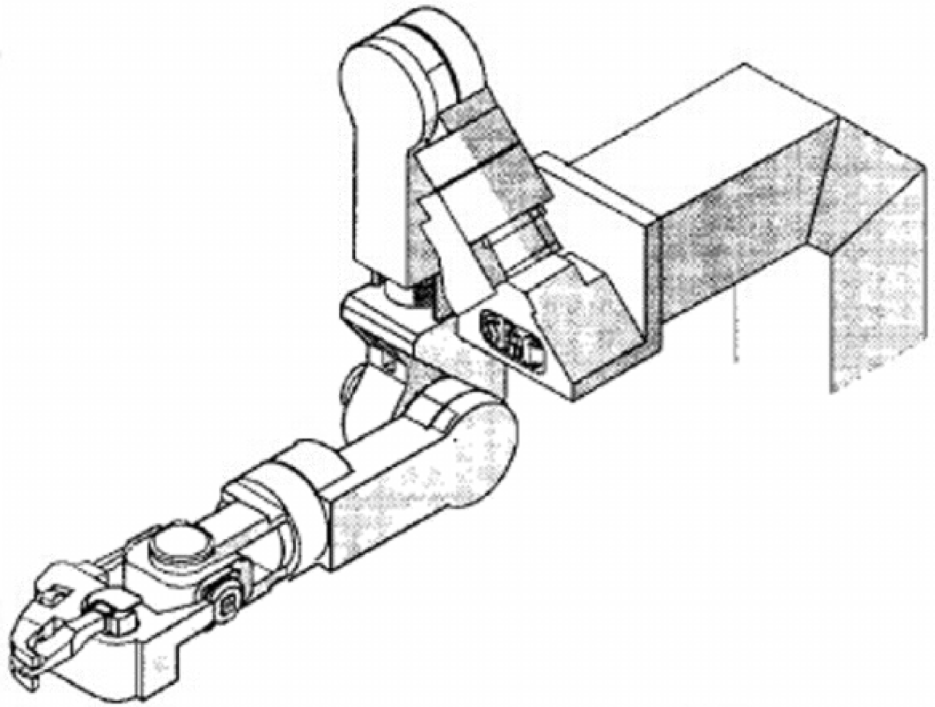
Original 1000 data points



Subsample of 128 data points

Subsampling Example - 7 Degree of Freedom SARCOS Robot Arm

- 21 total inputs:
  - 7 joint positions.
  - 7 joint velocities.
  - 7 joint accelerations.
  - 44,484 data points for the input space.
- 7 outputs are the joint torques.
- Subsample comparison:
  - Random subsample of 1,024 points.
  - SmartUQ subsample of the same size.

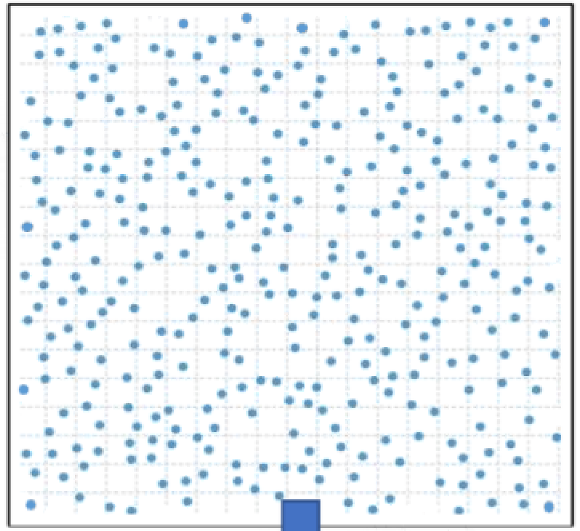


Source: Vijayakumar, S. and Schaal, S., 1997, "Local Dimensionality Reduction For Locally Weighted Learning", *CIRA '97 Proceedings.*

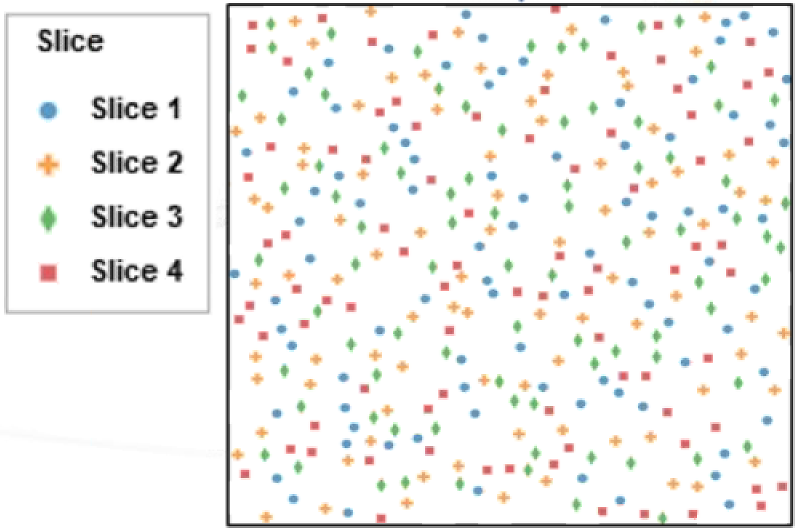
Data Source: http://www.gaussianprocess.org/gpml/data/

Unique to SmartUQ: Apportion Large Data Set into Several Data Slices

- **Slicing** apportions data into a user-desired number of data groups.
  - Each slice is representative of the entire domain
  - Generates multiple data sets for emulator training and model validation.
- Space Filling Composite Emulators use data slicing in a "divide and combine" training method.
- **Engineering Application:**
  - Allows for parallel computing, reducing computational times and eliminating memory roadblocks when solving engineering problems.



Original 1000 data points



Dataset, organized into 4 slices

Predictive Modeling (AKA Emulation, Surrogate Modeling)

SmartUQ

- Gaussian Process and many unique variants.
- Polynomial Chaos Expansion
- Response Surface Models
- Neural Networks
- Radial Basis Functions
- Generalized Linear Models
- Generalized Additive Models
- Stochastic Colocation

OpenTURNS

- Gaussian Process
- Polynomial Chaos Expansion
- Response Surface Models
- Taylor Expansions
- Mixture of Experts

SmartUQ Gaussian Process (GP) Model Advantages

- SmartUQ's GP models have been shown to train much faster than other commercial or open-source tools and with better accuracy.
- The GP tools in OpenTURNS can handle problems with continuous input and either continuous or functional output data. SmartUQ has many more unique GP model variants including for problems with:
  - Discrete or categorical inputs
  - Discrete response behavior
  - Spatially and/or temporally varying response
  - Large amounts of data
  - Large numbers of inputs

Gaussian Process (GP) Model Benchmark Example

- The training and validation data are from the *Rosenbrock Function*:
  - 15 independent features (inputs) uniformly distributed on the interval [-2,2].
  - The output is given by

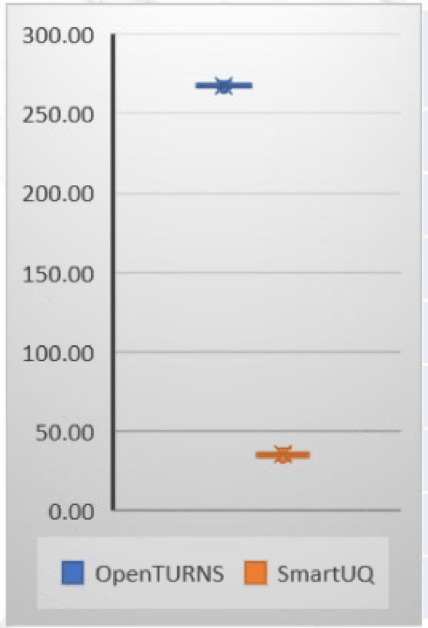
$$y(x) = \sum_{i=1}^{15} \left[100\left(x_{i+1} - x_i^2\right)^2 + (x_i - 1)^2\right]$$

- Benchmark was performed for Matérn kernel and two training set sizes (1000, 3000).
- Accuracies were checked using a 10,000 point validation set.
- For each training set size, the benchmark was repeated 10 times and statistics are reported on
  - Training time
  - RMSE on validation set

Training Time Comparison (Time in Seconds)

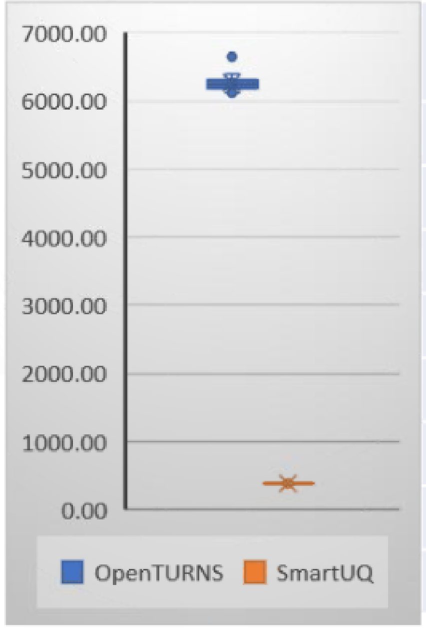
- Training time statistics are reported in seconds for the 10 replications of each model.
- SmartUQ's training times are MUCH faster than OpenTURNS.
- SmartUQ's slowest training time across the 10 replicates was faster OpenTURNS's fastest training time.

Training Samples: 1000



	OpenTURNS	SmartUQ
Minimum	265.86	31.96
5%	265.91	32.21
25%	267.08	34.12
50%	268.27	35.22
Mean	267.99	35.00
75%	268.81	35.79
95%	269.65	37.48
Maximum	270.00	38.77

Training Samples: 3000

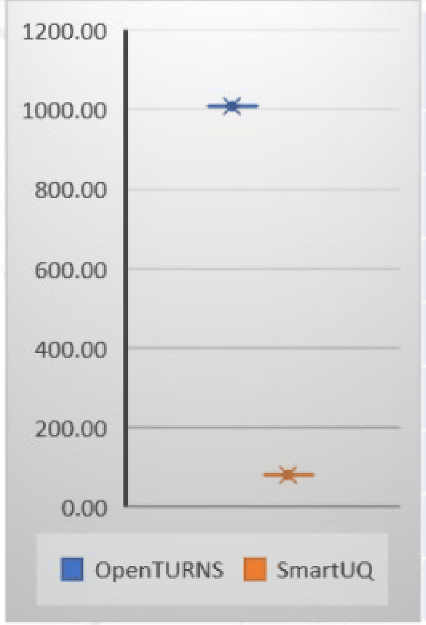


	OpenTURNS	SmartUQ
Minimum	6117.33	380.62
5%	6120.72	380.77
25%	6215.75	381.33
50%	6244.85	382.78
Mean	6274.74	383.91
75%	6272.34	384.70
95%	6532.75	390.27
Maximum	6649.69	393.23

Accuracy Comparison (Root Mean Square Error)

- SmartUQ's accuracy over the 10 replicates is far superior to OpenTURNS.
- SmartUQ's worst accuracy over the 10 replicates was MUCH better than OpenTURNS's best.
- As training set size increased SmartUQ's superiority in terms of accuracy also significantly increased.

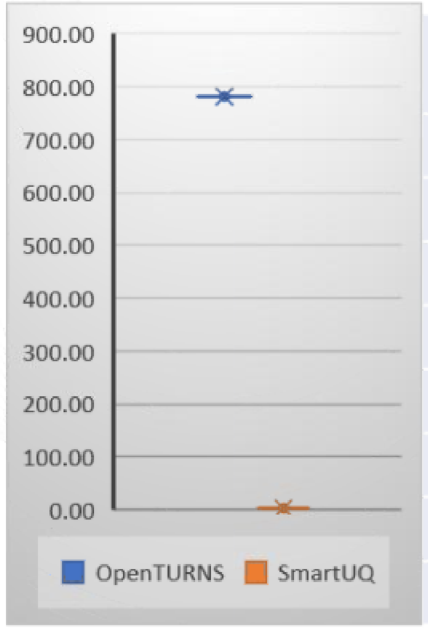
Training Samples: 1000



	OpenTURNS	SmartUQ
Minimum	1008.95	78.75
5%	1008.95	78.78
25%	1008.95	78.85
50%	1008.95	78.89
Mean	1008.95	78.90
75%	1008.95	78.97
95%	1008.95	79.05
Maximum	1008.95	79.08

RMSE of predictions on 10,000 sample validation set for the models trained with 1,000 samples.

Training Samples: 3000



	OpenTURNS	SmartUQ
Minimum	780.50	2.46
5%	780.50	2.46
25%	780.50	2.46
50%	780.50	2.46
Mean	780.50	2.46
75%	780.50	2.46
95%	780.50	2.46
Maximum	780.50	2.46

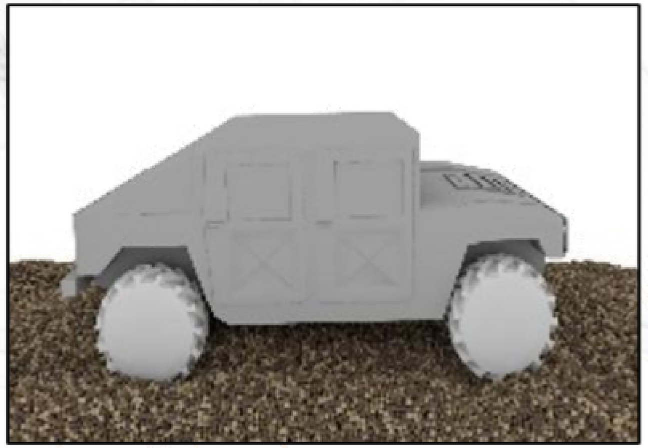
RMSE of predictions on 10,000 sample validation set for the models trained with 3,000 samples.

Gaussian Process Benchmark Summary

- **SmartUQ is faster:** SmartUQ's slowest training time across the 10 replicates was faster than OpenTURNS's fastest training time.
- **SmartUQ is more accurate:** SmartUQ's worst accuracy across the 10 replicates was better than OpenTURNS's best accuracy by a significant margin.
- **SmartUQ is superior for large data sets:** As data set size increased, SmartUQ's advantage over OpenTURNS in terms of accuracy also significantly increased.

All Models are Approximations of Reality

- *Modeling uncertainty* is the cumulative result of errors, assumptions, and approximations made when choosing the model.
  - *Model form uncertainty* is the uncertainty about the model's ability to capture the relevant system behaviors due to incomplete or inaccurate physical models.
  - *Parameter uncertainty* is the uncertainty about parameters within the model.



"Essentially, all models are wrong, but some are useful"

– George E. P. Box

Model Calibration

- Both SmartUQ and OpenTURNS have tools for model calibration.
- SmartUQ has
  - Data Matching (for continuous or functional response and continuous response with discrete/categorical inputs)
  - Frequentist Calibration
  - Bayesian Calibration (for continuous or functional response)
- OpenTURNS only has Bayesian calibration for continuous response.

Bayesian Calibration

SmartUQ

- Trains a surrogate of the simulation utilizing SmartUQ's superior GP models to account for nonlinear and more complex input-output relationships.
- Includes a discrepancy model to account for model form uncertainty (in addition to parameter uncertainty).
- Can be used for univariate continuous response, multivariate continuous response, and functional (e.g. time varying) response.

OpenTURNS

- Calibration must be performed directly on the simulation, i.e. no surrogate is trained. Consequently, calibration is only efficient enough to be possible for simulations that run very quickly (on the order of seconds).
- Does not consider discrepancy between the simulation and physical data it is being calibrated to. As such can only address parameter uncertainty.
- Can only be used for univariate and multivariate continuous response.

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SmartUQ

File | Data Exploration | DOE | Data Sampling | Automate | Validate | Calibrate | Emulate | Predict | Analytics | Help

LIBRARY

Search

- Bayesian Calibrated Emulator... $C^7 \rightarrow C^2$
- Bayesian Calibrated Emulator... $C^7 \rightarrow C^2$
- Physical Outputs 25 × 2
- Physical Inputs 25 × 7
- Bridge Results 100 × 2
- Bridge LHD 100 × 13

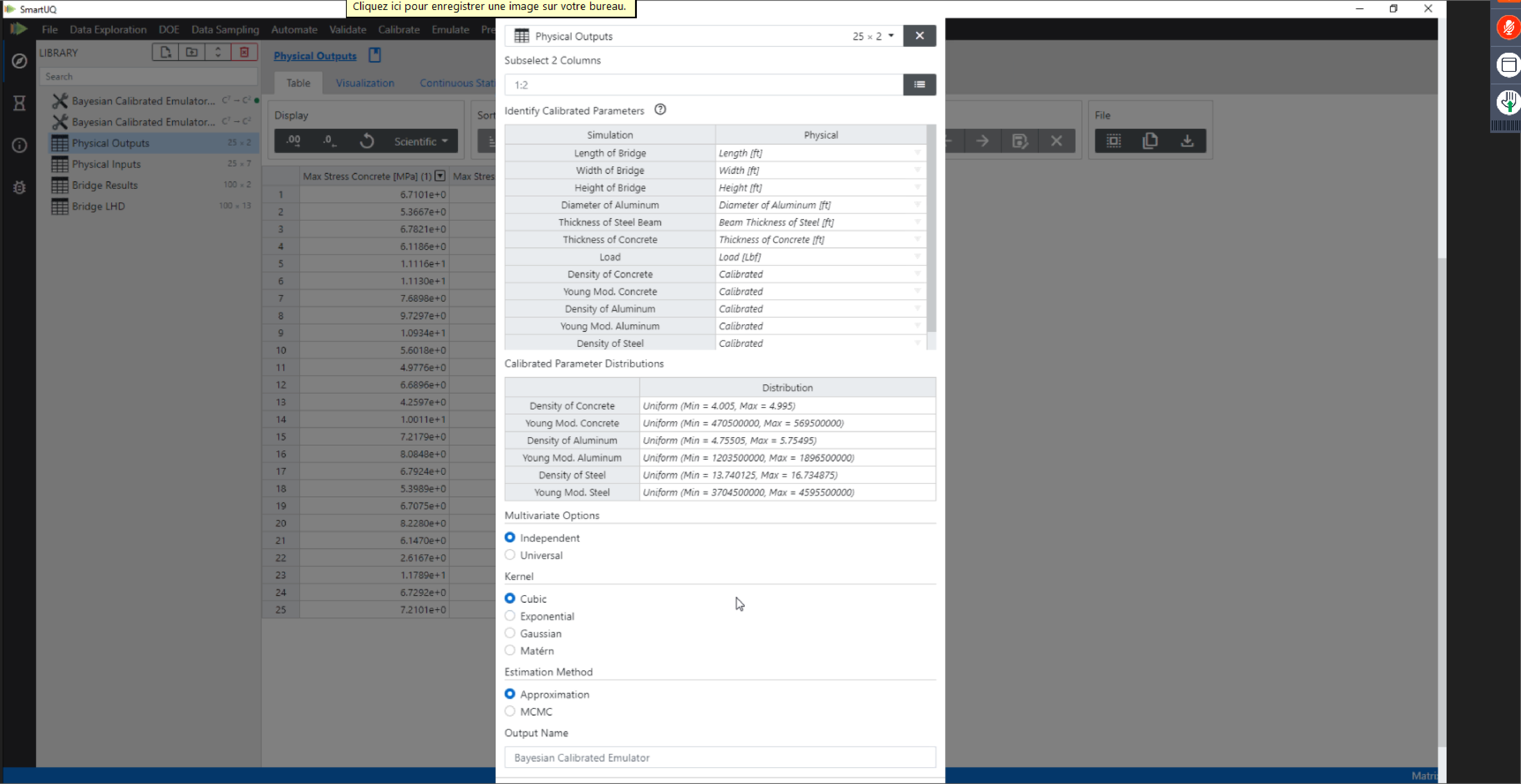
Bridge LHD

Table | Visualization | Continuous Statistics

Display: Scientific | Sort | Transform | Modify | Add | Edit | File

	Length of Bridge (1)	Width of Bridge (2)	Height of Bridge (3)	Diameter of Aluminum (4)	Thickness of Steel Beam (5)	Thickness of Concrete (6)	Load (7)	Density of Concrete (8)	Young Mod. Concrete (9)	Density of Aluminum (10
1	1.0500e+2	1.0660e+1	1.8840e+1	1.0602e-1	1.0162e-1	8.6500e-1	2.0180e+4	4.2450e+0	4.9150e+8	5.7448
2	1.0540e+2	1.0300e+1	2.2840e+1	7.9625e-2	1.2143e-1	6.9100e-1	2.0780e+4	4.7550e+0	5.0250e+8	5.1590
3	7.4200e+1	1.0180e+1	1.7800e+1	1.1373e-1	7.5225e-2	8.8900e-1	1.9620e+4	4.4450e+0	5.4450e+8	4.7752
4	9.7400e+1	9.7400e+0	1.8280e+1	7.5775e-2	1.0602e-1	4.1500e-1	1.9460e+4	4.7050e+0	5.5450e+8	4.9570
5	8.4200e+1	8.6200e+0	1.6360e+1	1.1482e-1	1.2198e-1	7.2100e-1	2.0260e+4	4.2250e+0	5.3250e+8	4.8964
6	7.4600e+1	1.1500e+1	2.1480e+1	9.2825e-2	8.4575e-2	8.3500e-1	2.1300e+4	4.0050e+0	5.5250e+8	5.5024
7	1.0900e+2	9.9400e+0	2.3720e+1	8.8975e-2	1.0328e-1	6.0700e-1	2.0140e+4	4.5050e+0	5.4150e+8	5.4216
8	9.3800e+1	8.9400e+0	1.6840e+1	7.9075e-2	8.2375e-2	5.2300e-1	2.0620e+4	4.1250e+0	5.0850e+8	4.9066
9	7.8200e+1	8.5800e+0	1.6040e+1	9.0075e-2	1.1263e-1	6.4300e-1	1.9660e+4	4.7650e+0	5.4850e+8	5.6742
10	7.6200e+1	1.0860e+1	1.7720e+1	8.9525e-2	1.2308e-1	5.8900e-1	2.1060e+4	4.3750e+0	5.6850e+8	5.0984
11	1.0060e+2	1.0420e+1	2.3320e+1	9.6125e-2	7.3025e-2	8.7700e-1	2.1020e+4	4.8950e+0	4.9550e+8	4.9470
12	8.5400e+1	9.9000e+0	1.8120e+1	1.0768e-1	9.2825e-2	7.5100e-1	1.8660e+4	4.3350e+0	5.5850e+8	5.1388
13	8.9800e+1	1.1300e+1	1.6280e+1	9.3375e-2	1.1482e-1	4.0300e-1	2.0100e+4	4.7850e+0	4.8950e+8	5.1288
14	8.2600e+1	8.2200e+0	2.3240e+1	8.1825e-2	1.1207e-1	4.3300e-1	2.1620e+4	4.6350e+0	4.9350e+8	5.5226
15	8.7400e+1	1.1460e+1	2.3640e+1	7.1925e-2	1.1317e-1	9.5500e-1	2.1180e+4	4.7350e+0	5.4050e+8	5.5428
16	9.1800e+1	1.1340e+1	2.3960e+1	9.2275e-2	1.2087e-1	6.2500e-1	1.8820e+4	4.5550e+0	5.5750e+8	4.9166
17	7.3800e+1	8.7800e+0	2.1560e+1	1.2362e-1	1.0272e-1	5.2900e-1	1.9140e+4	4.4550e+0	4.8550e+8	5.2196
18	9.7000e+1	9.4600e+0	1.7000e+1	9.7225e-2	9.9975e-2	9.7300e-1	1.8180e+4	4.8650e+0	5.3350e+8	4.7550
19	8.6600e+1	1.0820e+1	2.3480e+1	9.8325e-2	9.1725e-2	6.4900e-1	2.1700e+4	4.1450e+0	5.3750e+8	5.4722
20	9.0200e+1	8.4600e+0	1.8440e+1	1.1317e-1	9.6125e-2	9.1300e-1	1.8980e+4	4.3650e+0	4.9650e+8	5.5732
21	7.7800e+1	9.0200e+0	1.8600e+1	7.5225e-2	7.4675e-2	7.3300e-1	2.1980e+4	4.7450e+0	5.1850e+8	5.0076
22	9.8200e+1	9.1000e+0	2.3400e+1	1.2308e-1	1.0933e-1	7.0900e-1	1.8900e+4	4.9650e+0	4.7750e+8	5.4318
23	9.6200e+1	9.2600e+0	2.2280e+1	9.7775e-2	7.0275e-2	4.5100e-1	2.0420e+4	4.0550e+0	5.5050e+8	5.3610
24	8.2200e+1	9.5400e+0	2.0680e+1	9.6675e-2	1.2033e-1	4.2700e-1	1.9380e+4	4.3950e+0	4.7450e+8	5.6236
25	1.0140e+2	8.7000e+0	1.8920e+1	8.2375e-2	7.1925e-2	6.6700e-1	1.8380e+4	4.5850e+0	5.6650e+8	5.3106
26	1.0820e+2	9.7000e+0	2.2520e+1	1.2198e-1	9.2275e-2	9.0700e-1	2.1900e+4	4.3450e+0	5.1950e+8	5.3510
27	1.0300e+2	9.3000e+0	1.8040e+1	1.1593e-1	1.1922e-1	8.1100e-1	2.1660e+4	4.5350e+0	5.0750e+8	5.6540
28	9.2200e+1	1.0980e+1	1.9480e+1	1.1538e-1	1.0712e-1	9.9100e-1	1.8740e+4	4.6450e+0	5.1750e+8	5.4520
29	7.5800e+1	9.7800e+0	1.8200e+1	1.2473e-1	8.0175e-2	5.7700e-1	1.8260e+4	4.6650e+0	5.3550e+8	4.8762
30	1.0660e+2	1.1700e+1	1.6200e+1	1.0053e-1	9.4475e-2	5.1700e-1	1.8860e+4	4.4350e+0	5.5550e+8	5.4418
31	1.0380e+2	8.9000e+0	1.7560e+1	1.0383e-1	9.0625e-2	9.8500e-1	1.9740e+4	4.1950e+0	5.6050e+8	5.2500
32	1.0100e+2	8.9800e+0	2.1320e+1	1.0933e-1	1.2362e-1	4.6900e-1	1.9300e+4	4.6950e+0	5.3650e+8	5.4822
33	8.5000e+1	9.2200e+0	1.6760e+1	1.1978e-1	1.0823e-1	6.0100e-1	1.9420e+4	4.2550e+0	4.8150e+8	5.0176

Matrix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Calibrate
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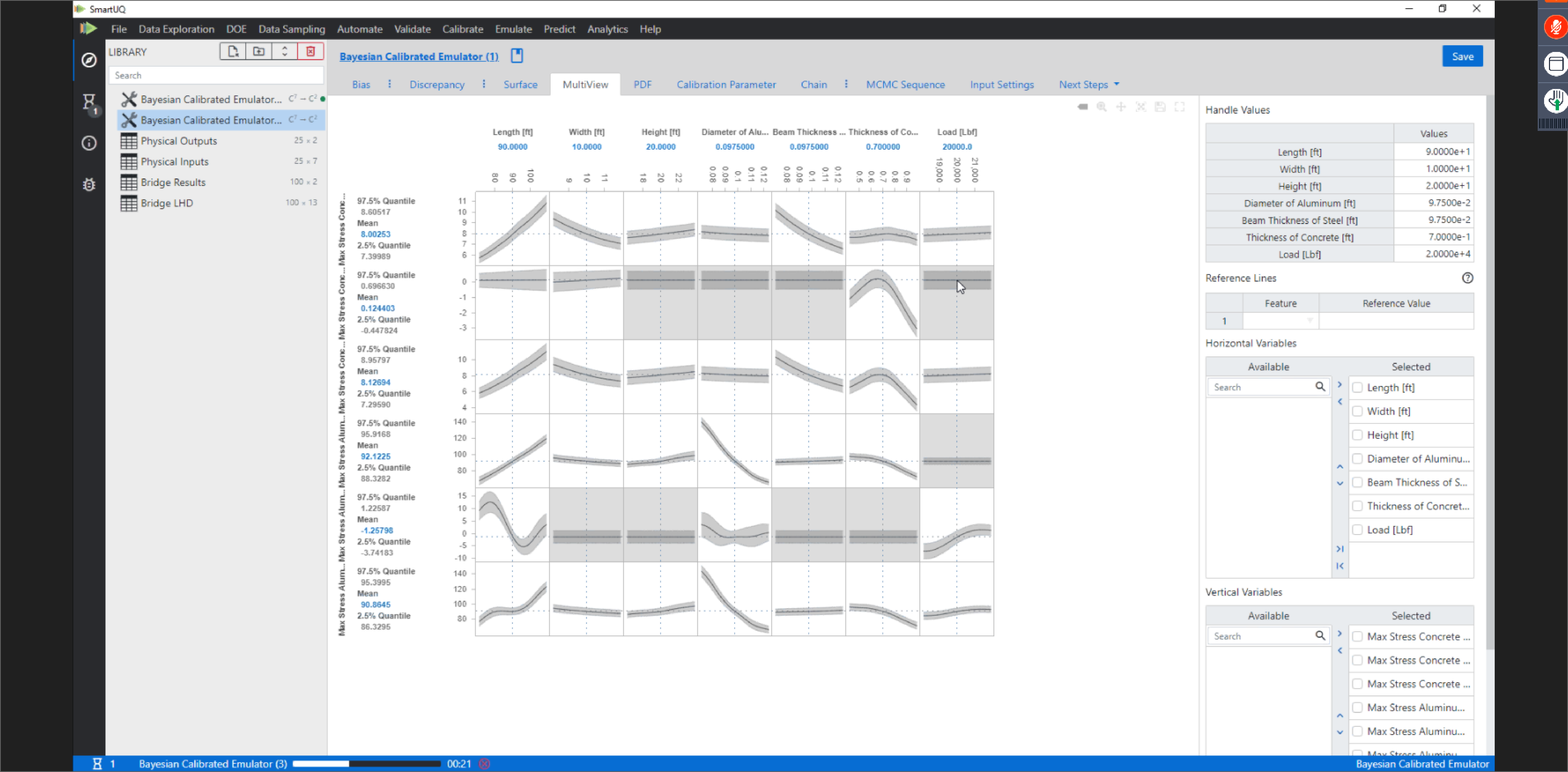
Search
Bayesian Calibrated Emulator...
Bayesian Calibrated Emulator...
Physical Outputs 25 × 2
Physical Inputs 25 × 7
Bridge Results 100 × 2
Bridge LHD 100 × 13
Physical Outputs
Table
Visualization
Continuous Stat
Display
Scientific
Sort
File
Max Stress Concrete [MPa] (1)
1 6.7101e+0
2 5.3667e+0
3 6.7821e+0
4 6.1186e+0
5 1.1116e+1
6 1.1130e+1
7 7.6898e+0
8 9.7297e+0
9 1.0934e+1
10 5.6018e+0
11 4.9776e+0
12 6.6896e+0
13 4.2597e+0
14 1.0011e+1
15 7.2179e+0
16 8.0848e+0
17 6.7924e+0
18 5.3989e+0
19 6.7075e+0
20 8.2280e+0
21 6.1470e+0
22 2.6167e+0
23 1.1789e+1
24 6.7292e+0
25 7.2101e+0
Physical Outputs 25 × 2
Subselect 2 Columns
1:2
Identify Calibrated Parameters
Simulation | Physical
Length of Bridge | Length [ft]
Width of Bridge | Width [ft]
Height of Bridge | Height [ft]
Diameter of Aluminum | Diameter of Aluminum [ft]
Thickness of Steel Beam | Beam Thickness of Steel [ft]
Thickness of Concrete | Thickness of Concrete [ft]
Load | Load [Lbf]
Density of Concrete | Calibrated
Young Mod. Concrete | Calibrated
Density of Aluminum | Calibrated
Young Mod. Aluminum | Calibrated
Density of Steel | Calibrated
Calibrated Parameter Distributions
Distribution
Density of Concrete | Uniform (Min = 4.005, Max = 4.995)
Young Mod. Concrete | Uniform (Min = 470500000, Max = 569500000)
Density of Aluminum | Uniform (Min = 4.75505, Max = 5.75495)
Young Mod. Aluminum | Uniform (Min = 1203500000, Max = 1896500000)
Density of Steel | Uniform (Min = 13.740125, Max = 16.734875)
Young Mod. Steel | Uniform (Min = 3704500000, Max = 4595500000)
Multivariate Options
Independent
Universal
Kernel
Cubic
Exponential
Gaussian
Matérn
Estimation Method
Approximation
MCMC
Output Name
Bayesian Calibrated Emulator


SmartUQ
File
Data Exploration
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Data Sampling
Automate
Validate
Calibrate
Emulate
Predict
Analytics
Help
LIBRARY
Search
Bayesian Calibrated Emulator...
Bayesian Calibrated Emulator...
Physical Outputs 25 × 2
Physical Inputs 25 × 7
Bridge Results 100 × 2
Bridge LHD 100 × 13
Bayesian Calibrated Emulator (1)
Save
Bias
Discrepancy
Surface
MultiView
PDF
Calibration Parameter
Chain
MCMC Sequence
Input Settings
Next Steps
Length [ft]
90.0000
Width [ft]
10.0000
Height [ft]
20.0000
Diameter of Alu...
0.0975000
Beam Thickness ...
0.0975000
Thickness of Co...
0.700000
Load [Lbf]
20000.0
97.5% Quantile
8.60517
Mean
8.00253
2.5% Quantile
7.39989
97.5% Quantile
0.696630
Mean
0.124403
2.5% Quantile
-0.447824
97.5% Quantile
8.95797
Mean
8.12694
2.5% Quantile
7.29590
97.5% Quantile
95.9168
Mean
92.1225
2.5% Quantile
88.3282
97.5% Quantile
1.22587
Mean
-1.25798
2.5% Quantile
-3.74183
97.5% Quantile
95.3995
Mean
90.8645
2.5% Quantile
86.3295
Handle Values
Values
Length [ft] 9.0000e+1
Width [ft] 1.0000e+1
Height [ft] 2.0000e+1
Diameter of Aluminum [ft] 9.7500e-2
Beam Thickness of Steel [ft] 9.7500e-2
Thickness of Concrete [ft] 7.0000e-1
Load [Lbf] 2.0000e+4
Reference Lines
Feature
Reference Value
Horizontal Variables
Available
Selected
Search
Length [ft]
Width [ft]
Height [ft]
Diameter of Aluminu...
Beam Thickness of S...
Thickness of Concret...
Load [Lbf]
Vertical Variables
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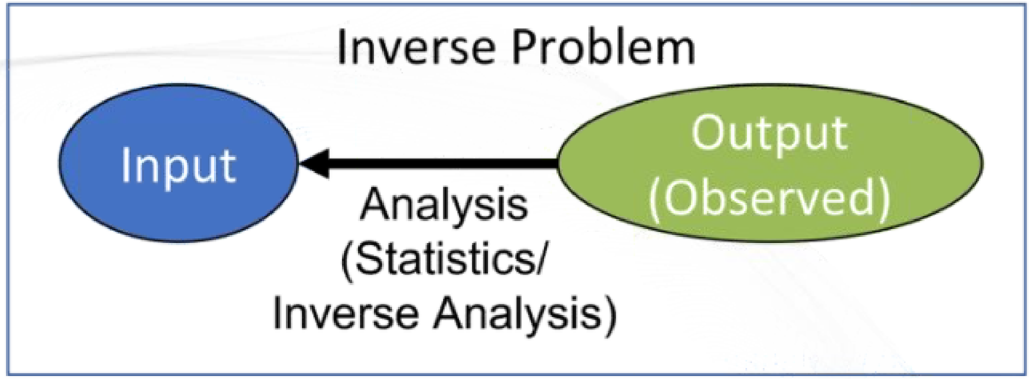
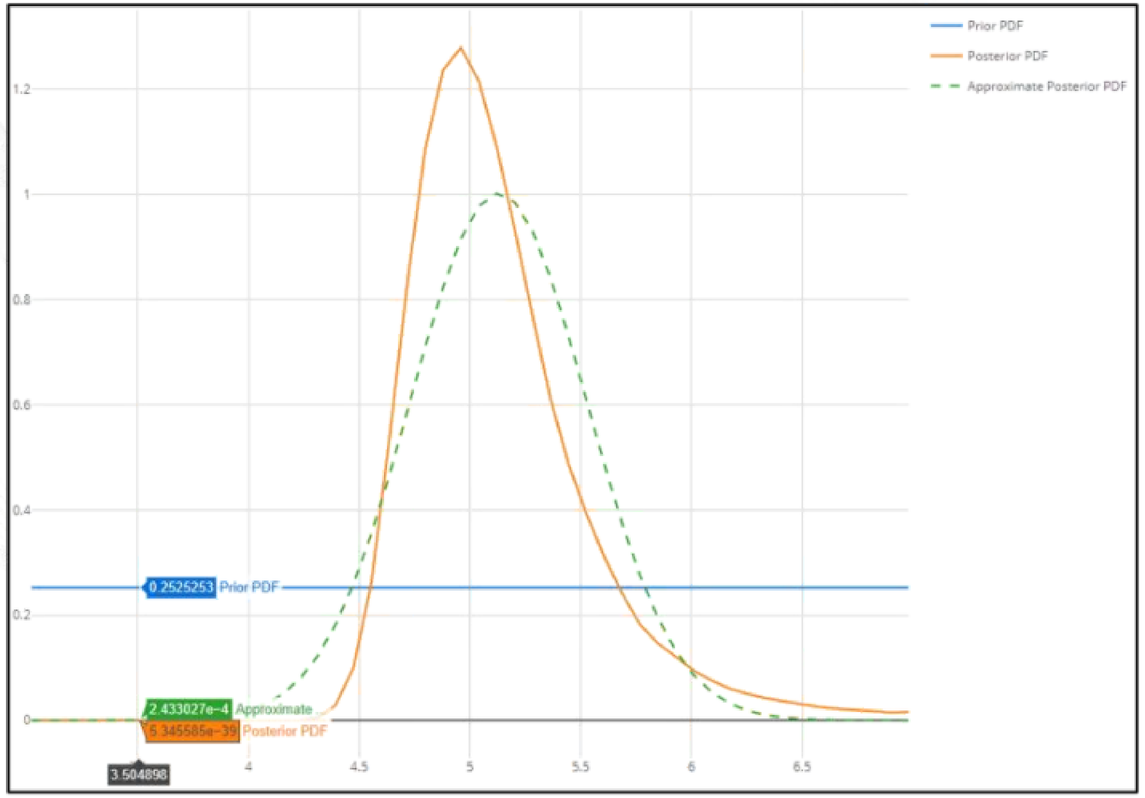
Selected
Search
Max Stress Concrete ...
Max Stress Concrete ...
Max Stress Concrete ...
Max Stress Aluminu...
Max Stress Aluminu...
Bayesian Calibrated Emulator (3)
00:21
Bayesian Calibrated Emulator

Unique to SmartUQ: Inverse Analysis

- Inverse analysis characterizes the uncertainty in unobserved inputs based on observed outputs.
- Finds the most likely input distributions which yield the observed outputs.
- SmartUQ has both a frequentist and Bayesian option for Inverse Analysis.





Other Differences

- Sensitivity Analysis (SA)
  - SmartUQ performs global SA for problems with either continuous or functional response
  - SmartUQ has tools for visualization of local sensitivity analysis
  - OpenTURNS performs global SA for continuous response problems only
- Uncertainty Propagation (UP)
  - SmartUQ handles cases of aleatory, epistemic, and mixed (aleatory and epistemic) uncertainty
  - OpenTURNS only handles aleatory uncertainty
- SmartUQ has PCA for dimension reduction
- SmartUQ has both a user-friendly GUI and Python API, while OpenTURNS can only be used via Python programming.
- SmartUQ includes Stochastic and reliability-based optimization (RBO) tools for solving optimization problems under uncertainty

SmartUQ Simulation Integration and Automation Tools

- SmartUQ can be linked to simulation tools
  - Allows SmartUQ to retrieve parameter information from the model (useful for easy DOE creation)
  - From within SmartUQ, simulations for example from a DOE, can be sent directly to linked model for evaluation. Results are automatically returned to SmartUQ.

Integration Tools

- GUI Tools Specific to:
  - ANSYS Workbench
  - Adams View and Car
  - COMSOL
- Command Line Simulation:
  - SmartUQ can connect to any simulation model or data source located on the computer by calling it through the computer's command line.
- SmartSim I/O:
  - Reads and writes directly from files used by the external simulation software, rather than using an input/output wrapper like the Command Line Simulation tool.
  - Coupled with advanced text parsing tools making it possible to quickly set up and run simulation models.

SmartUQ Simulation Integration and Automation Tools

Automation Tools (make use of linked simulation models)

- Dynamic Emulation:
  - User defines an accuracy target for the surrogate model and a maximum number of simulation runs allowed to reach the target.
  - SmartUQ will follow a fully automated iterative process of running simulations, collecting results, training the model, and assessing model accuracy, until either targeted accuracy threshold or maximum samples is reached.
- Dynamic Optimization:
  - Automated process to optimize objective function associated with the simulation
  - Samples are iteratively run through the simulation, an emulator trained, and the emulator used to select the next simulations to run.

More Information…

- **Upcoming Webinars:**
  – **February 22, 2023:** Introduction to SmartUQ Machine Learning Software, by Gavin Jones, SmartUQ Pr. Application Engineer
- **Download SmartUQ white papers from our website:** http://www.smartuq.com/resources/whitepaper/
  – *Statistical Calibration: Grounding Simulations in Reality*
  – *Introduction to SmartUQ analytics and Digital Twins*
- **On Demand Webinars:** http:// smartuq.com/resources/webinars
  – *Machine Learning and Uncertainty Quantification for Engineering Simulation*
  – *Machine Learning for Narrowing the Simulation-Test Gap*