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Dakota Integrated with MFiX for UQ Analysis: Sensitivity of particle size on pressure drop in a fluidized bed DEM simulations

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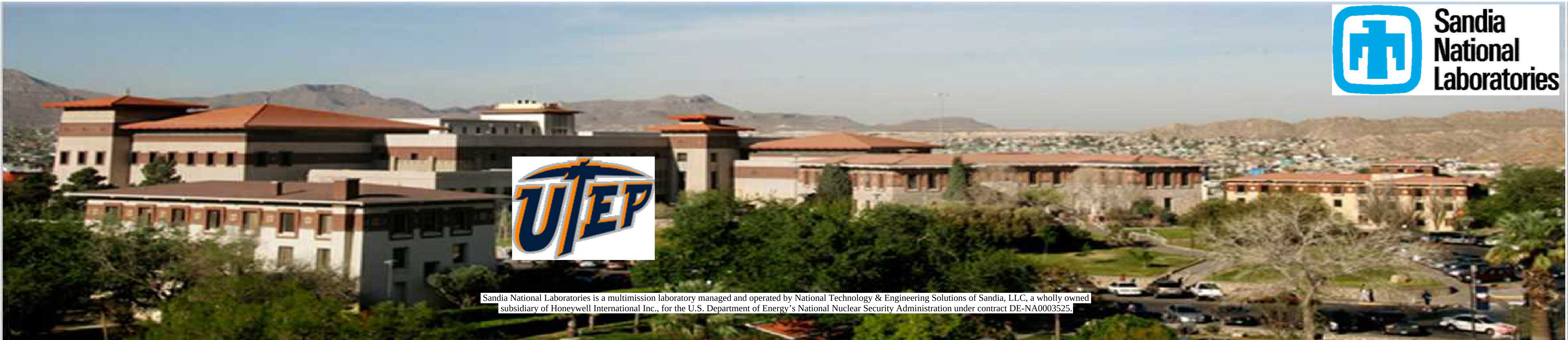

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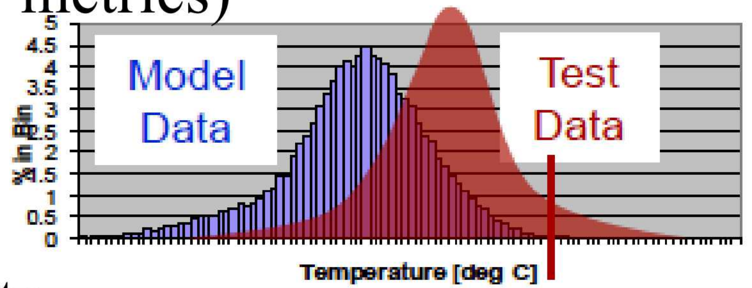
Why Uncertainty Quantification?

What? Determine variability, distributions, statistics of code outputs, given uncertainty in input factors; put error bars on simulation output

Why? Tactically, assess likelihood of typical or extreme outcomes. Given input uncertainty…

- Determine mean or median performance of a system
- Assess variability or robustness of model response
- Find probability of reaching failure/success criteria (reliability metrics)
- Assess range/intervals of possible outcomes



Ultimately, use simulations for risk-informed decision making, e.g., assess how close uncertainty-endowed code predictions are to

- Experimental data (validation, is model sufficient for the intended application?)
- Performance expectations or limits (quantification of margins and uncertainties; QMU)

A Practical Process for UQ

1. Determine UQ analysis goals
- Identify the key model responses (quantities of interest)
- What kind of statistics or metrics do we want on them?

2. Identify potentially influential uncertain input parameters
- Includes parameters that influence trend in response as well as those that influence variability in response

3. Characterize input uncertainties and map them into Dakota variable specifications

4. What are the model characteristics/behaviors?
- Simulation cost, model robustness, input/output properties such as kinks, discontinuities, multi-modal, noise, disparate regimes

5. Select a method appropriate to variables, goal, and problem

6. Set up Dakota input file and interface to simulation

7. Run study and interpret the results

Key Statistics Ideas: Moments of Random variables

Understanding the following basic concepts will help with Dakota UQ

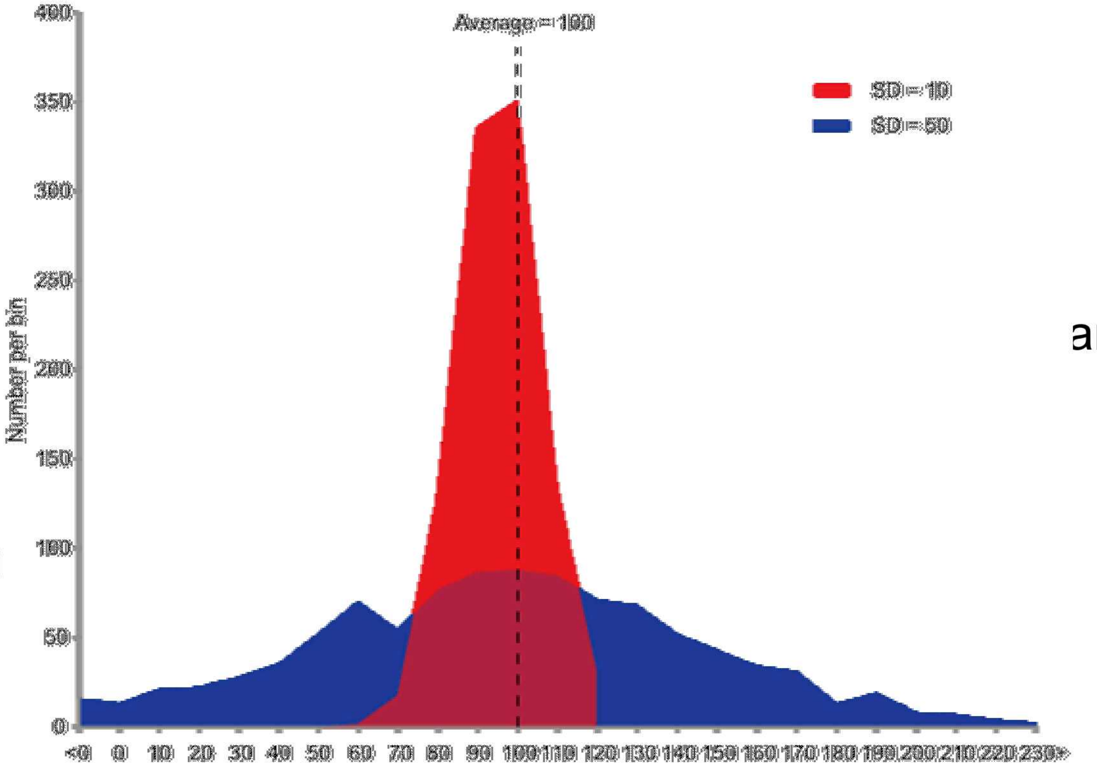
Concept of a random variable *X*

Mean (*m*, *μ*): expected or average value of *X*, *e.g., mean of sample of size N:*

$\mu_x = \frac{1}{N} \sum_{i=1}^{N} x^i$

Standard deviation (*s*, *σ*): measure of dispersio / variability of *X:*

$\sigma_T = \sqrt{\frac{1}{N} \sum_{i=1}^{N} [(x^i) - \mu_x]^2}$



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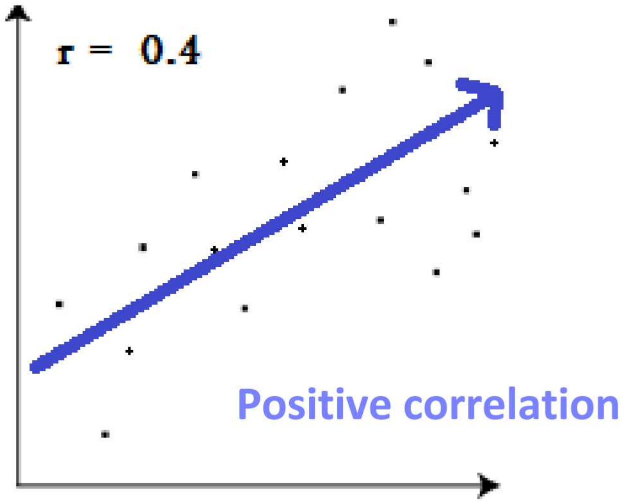
Key Statistics Ideas: correlation coefficients

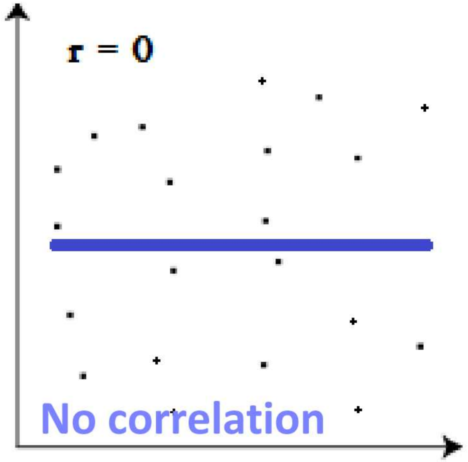
- **Correlation coefficients** are used in statistics to measure how strong a relationship is between two variables. There are several types of correlation coefficient: Pearson's correlation (also called Pearson's *R*) is a **correlation coefficient** commonly used in linear regression
- Correlation coefficient formulas are used to find how strong a relationship is between data. The formulas return a value between -1 and 1

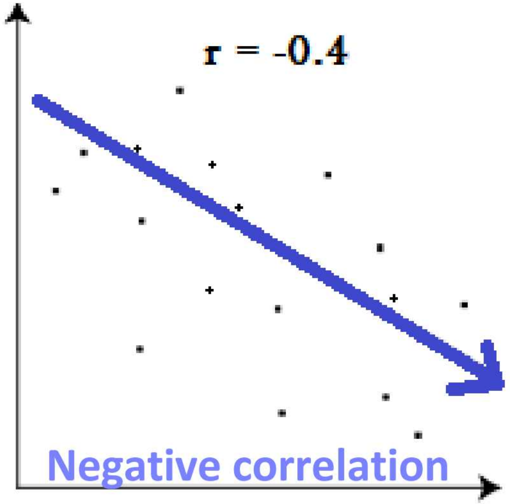
✓1 indicates a strong positive relationship.

✓-1 indicates a strong negative relationship.

✓A result of zero indicates no relationship at all.

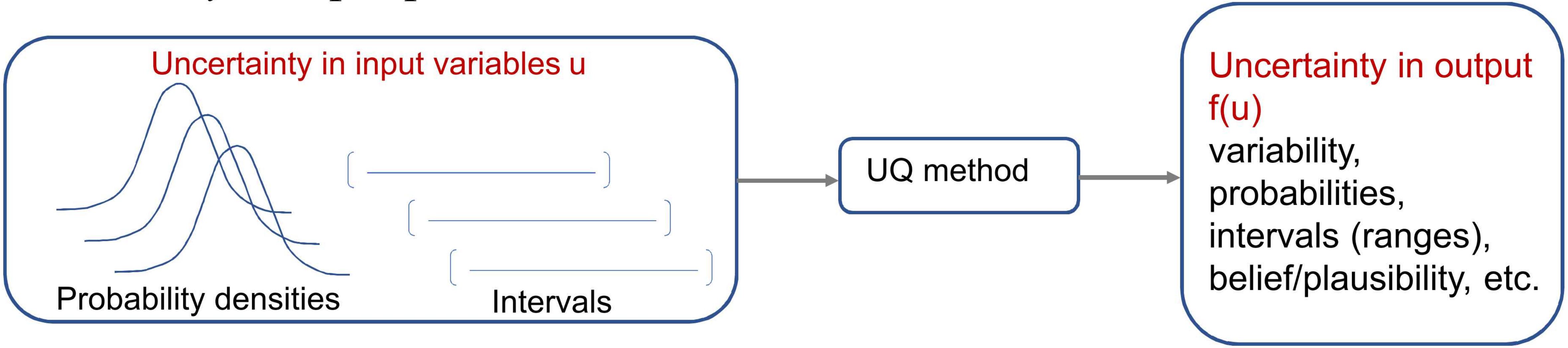






Dakota Uncertainty Quantification

- Dakota UQ methods primarily focus on forward propagation of parametric uncertainties through a model: *determine uncertainty in* model output, given uncertai*nty in input parameters*



- Example uncertain inputs: physics parameters, material properties boundary/initial conditions, operating conditions, model choice, geometry
- Can also perform "inverse UQ" to determine uncertainties in parameters consistent with data

Selecting a UQ method

Consider variable characterizations, model properties, ultimate UQ goal to choose a method

Sampling (Monte Carlo, LHS)
- ✓ Robust, understandable, and applicable to most any model
- ✓ Slow to converge
- ✓ Moments, PDF/CDF, correlations, min/max

Stochastic Expansions
- ✓ Surrogate models tailored to UQ for continuous variables
- ✓ Highly efficient for smooth model responses
- ✓ Moments, PDF/CDF, Sobol indices

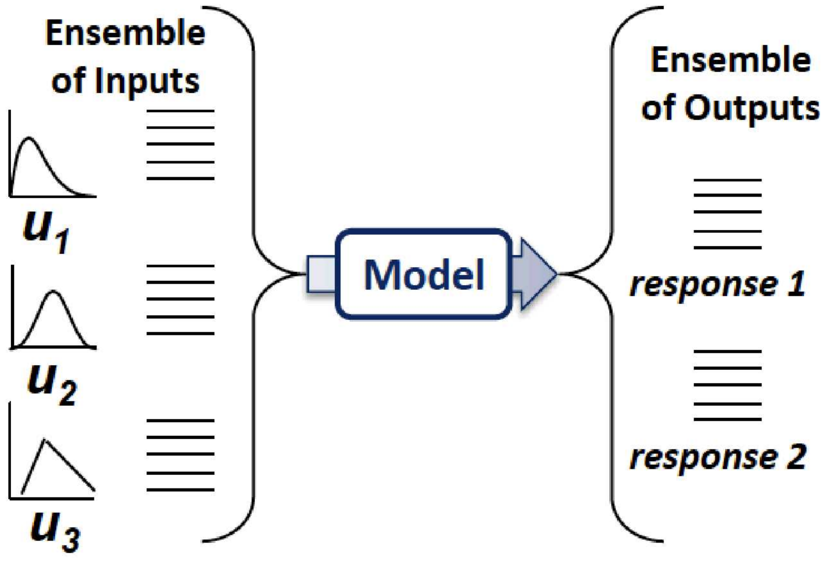
Reliability
- Goal-oriented; target particular response or probability levels
- Efficient local (require derivatives) / global variants
- Moments, PDF/CDF, importance factors

Epistemic
- Non-probabilistic methods
- Generally applicable, can be costly when no surrogate
- Belief/plausibility, intervals, probability of frequency

Monte Carlo Sampling (MCS)

Sampling methods draw (pseudo-random) realizations from the specified input distributions, run the simulation, and calculate sample statistics:

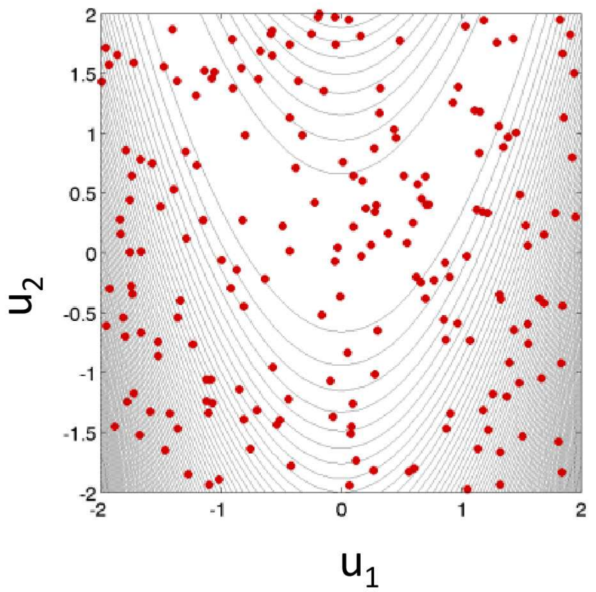
- ✓ Sample moments, min/max, empirical PDF/CDF, based on ensemble of calculations



Robust even for complex, poorly-behaved simulations

Slow, though reliable convergence: **$O(N^{-1/2})$**, (in theory) independent of dimension

Latin Hypercube Sampling (LHS)



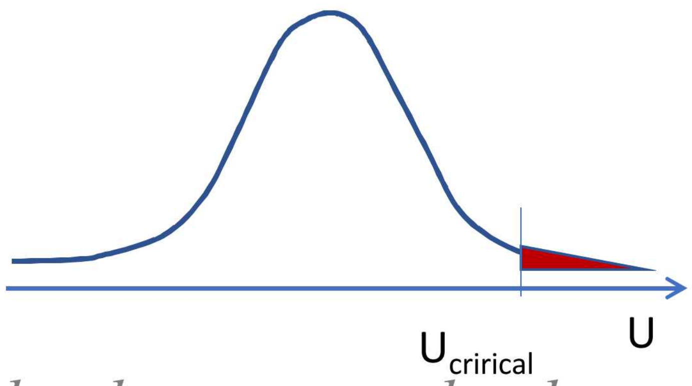
Dakota has *sample_type* options random and lhs

- ✓LHS is recommended when possible
- ✓Better convergence rate and stability across replicates
- ✓Any follow-on studies must double the sample size
- ✓LHS (McKay and Conover): stratified random sampling among equal probability bins for all 1-D projections of an n-dimensional set of samples

Reliability Methods

Goal-oriented methods that focus on regions of probability or response space of interest, for example:

- What temperature is achieved with 99% probability?
- What is the probability of exceeding $U_{critical}$?



Naïve sampling can be ineffective / under-resolved

- Run 10,000 samples, only 5 are in relevant region

Need to specify to Dakota

- Probability or response threshold(s) of interest using *probability_levels*, *response_levels*

Method choice

- Mean-value: best for linear problems, normally distributed parameters, efficient derivatives; specify *local_reliability* (with no mpp_search)
- MPP: computes most probable point of failure when failure boundary is near linear or quadratic; specify *local_reliability* (with an mpp_search option)
- Adaptive: computes probability of failure for complicated failure boundaries; specify *global_reliability*

Stochastic Expansions

General-purpose UQ methods that build UQ-tailored polynomial approximations of the output responses

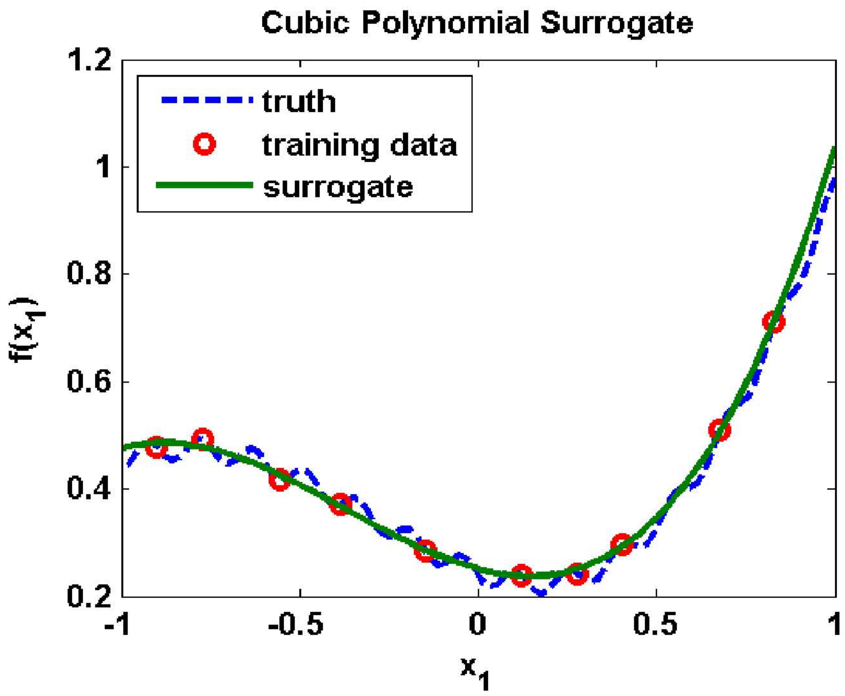
Perform particularly well for smooth model responses

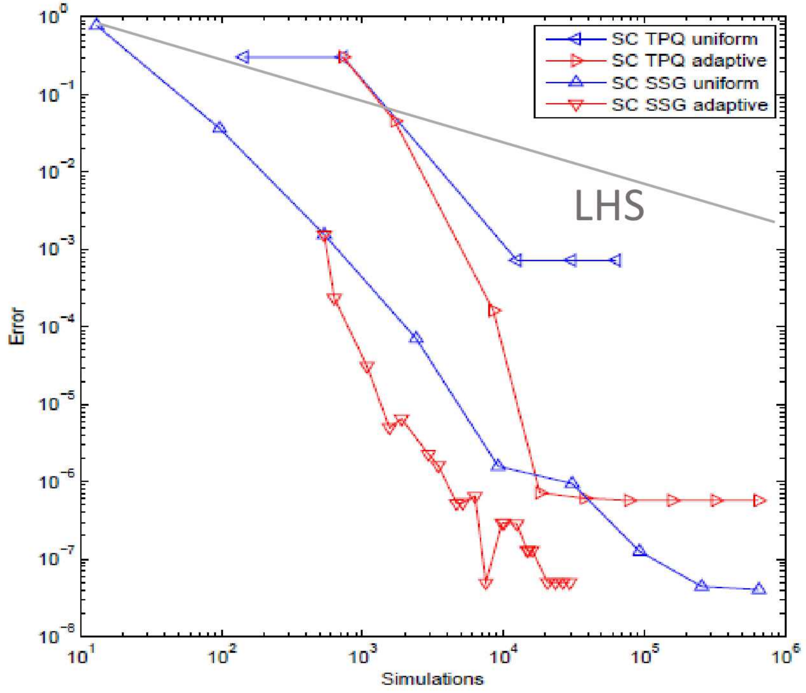
Resulting convergence of statistics can be considerably faster than sampling methods

Need to specify the Dakota method:

✓ **Polynomial Chaos (polynomial_chaos):** specify the type of orthogonal polynomials and coefficient estimation scheme, e.g., sparse grid or linear regression.

- **Stochastic Collocation (stoch_collocation):** specify the type of polynomial basis and the points at which the response will be interpolated; supports piecewise local basis





Dakota UQ Methods Summary

Character	Method class	Problem character	Variants
aleatory	**probabilistic sampling**	**nonsmooth, multimodal, modest cost, #variables**	**Monte Carlo, LHS, importance**
	local reliability	smooth, unimodal, more variables, failure modes	mean value and MPP, FORM/SORM
	global reliability	nonsmooth, multimodal, low dimensional	EGRA
	stochastic expansions	**nonsmooth, multimodal, low dimension**	**polynomial choas, stochastic collocation**
Epistemic	Interval estimation	sample intervals	global/local optimization, sampling
	evidence theory	belief structures	global/local evidence
both	nested UQ	mixed aleatory/epistemic	nested

UQ results with Dakota

MCS with 100,000 samples

Case #	Input1 $e_{p,n}$	Input 2 $e_{w,n}$	Bed height Sample mean	Bed height Sample Std deviation
1	N(0.8,0.1)	N(0.8,0.1)	14.37	1.7e-01
2	N(0.8,0.1)	N(0.8,0.05)	14.37	1.6e-1

Flow in the fluidized bed

$e_{p,n}$ = particle-particle restitution co-efficient

$e_{w,n}$ = Particle-wall restitution co-efficient

UQ results with PSUADE

MCS with 100,000 samples

Case #	Input1 $e_{p,n}$	Input 2 $e_{w,n}$	Bed height Sample mean	Bed height Sample Std deviation
1	N(0.8,0.1)	N(0.8,0.1)	14.37	1.7e-1
2	N(0.8,0.1)	N(0.8,0.05)	14.37	1.5e-1

Response function (Bed height) =

$$= 17.026 - 7.767\, e_{p,n} - 0.46428 e_{w,n} + 5.6644\, e_{p,n}^2 + 0.18379\, e_{p,n}\, e_{w,n} + 0.20556\, e_{w,n}^2$$

Surrogate model

Gel, A., Garg, R., Tong, C., Shahnam, M. and Guenther, C., 2013. Applying uncertainty quantification to multiphase flow computational fluid dynamics. *Powder technology*, *242*, pp.27-39.

UQ results with Dakota

MCS with 100,000 samples

Case #	Input1 $e_{p,n}$	Input 2 $e_{w,n}$	Bed height Sample mean	Bed height Sample Std deviation
1	N(0.8,0.1)	N(0.8,0.1)	14.374	1.7e-01
2	N(0.8,0.05)	N(0.8,0.1)	14.332	7.5e-2
3	N(0.8,0.1)	N(0.8,0.05)	14.372	1.6e-1
4	N(0.8,0.05)	N(0.8,0.05)	14.330	7.5e-2

$e_{p,n}$ = particle-particle restitution co-efficient

$e_{w,n}$ = Particle-wall restitution co-efficient

Response function - bed height(h) =

$$= 17.026 - 7.767\, e_{p,n} - 0.46428 e_{w,n} + 5.6644\, e_{p,n}^2 + 0.18379\, e_{p,n}\, e_{w,n} + 0.20556\, e_{w,n}^2$$

PCE (order =5) with different standard deviation specifications for input parameter distributions.

Case #	Input1 $e_{p,n}$	Input 2 $e_{w,n}$	Bed height Sample mean	Bed height Sample Std deviation
1	N(0.8,0.1)	N(0.8,0.1)	14.374	1.7e-01
2	N(0.8,0.05)	N(0.8,0.1)	14.332	7.5e-2
3	N(0.8,0.1)	N(0.8,0.05)	14.372	1.6e-1
4	N(0.8,0.05)	N(0.8,0.05)	14.330	7.5e-2

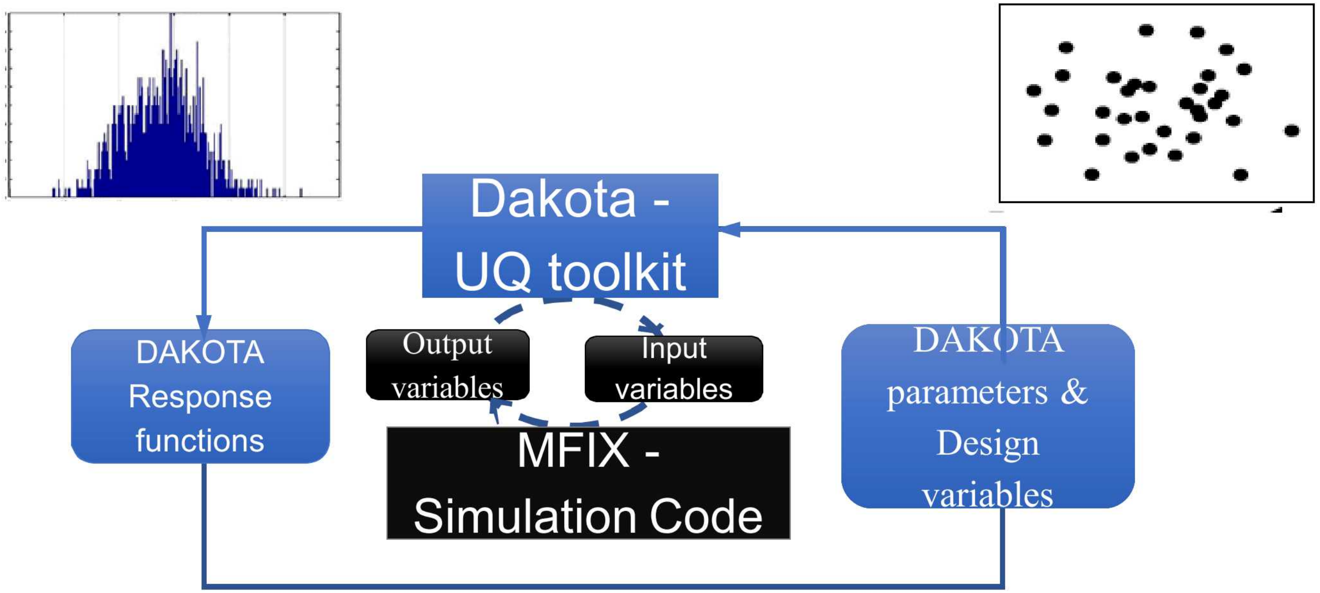
UQ results with Dakota

MCS– sample size study

samples	Input1 $e_{p,n}$	Input 2 $e_{w,n}$	h mean	h Std deviation
100,000	N(0.8,0.1)	N(0.8,0.1)	14.374	1.65e-01
10,000	N(0.8,0.1)	N(0.8,0.1)	14.374	1.65e-01
1000	N(0.8,0.1)	N(0.8,0.1)	14.374	1.65e-01
500	N(0.8,0.1)	N(0.8,0.1)	14.374	1.65e-01
200	N(0.8,0.1)	N(0.8,0.1)	14.374	1.66e-01
100	N(0.8,0.1)	N(0.8,0.1)	14.376	1.73e-01
50	N(0.8,0.1)	N(0.8,0.1)	14.372	1.59e-01
20	N(0.8,0.1)	N(0.8,0.1)	14.363	1.40e-01
10	N(0.8,0.1)	N(0.8,0.1)	14.356	1.32e-01

Implementation of MFiX in Dakota

- In order to create an interface between the two independent software packages, a **c++ wrapper is created**. This wrapper facilitates interaction between Dakota and MFIX.
- In the current workflow model, **Dakota is the primary driver**, i.e., Dakota performs the preparations, and then performs the uncertainty quantification via the response functions **returned from the wrapper for MFiX** results. In a separate input file for Dakota, the user prescribes the variables with uncertainty and a range of values to determine the upper and lower bounds.
- Quantities of interest or response variables with the type of UQ analysis to be performed are also specified in this input file.



Schematic of a loosely-coupled or "black-box" interface between Dakota and MFiX – a multiphase CFD solver

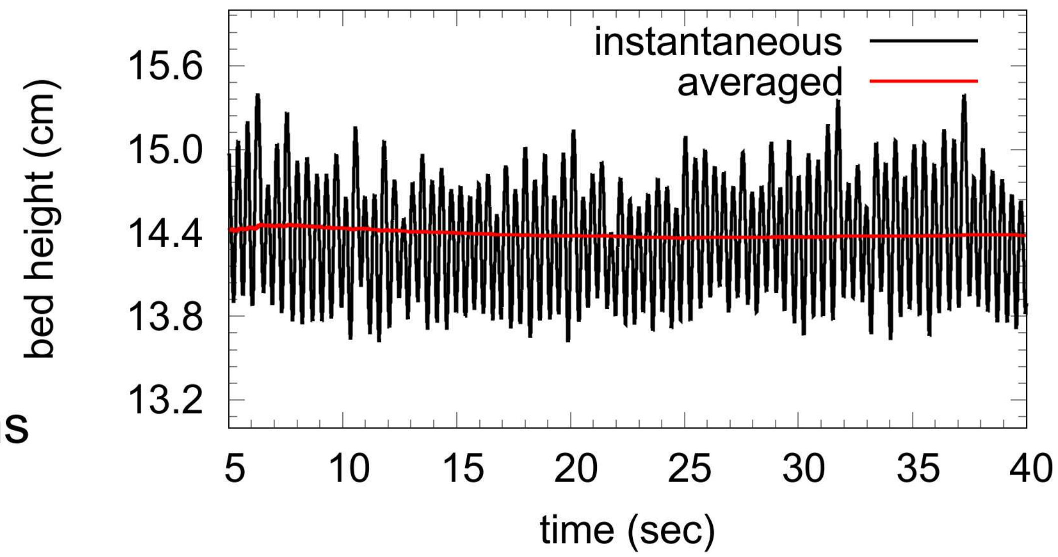
Implementation of MFiX in Dakota

- The C++ wrapper creates **separate work directories for each independent run** and **modifies the input file for MFiX simulations** by substituting new set of values for the variables that were prescribed by the user to be treated as uncertain or varied if employing design of experiments. The values for these variables are determined based on several factors such as the sampling method chosen, number of samples, upper and lower bounds and the probability distribution function prescribed for the uncertain variable(s) in the Dakota input file.
- **The Wrapper launches MFiX executable for each sample independently**
- **Once the simulation is completed, the response functions values from MFiX is returned to Dakota** for uncertainty analysis such as sensitivity study, or propagating uncertainties to determine their effect on the quantities of interest.

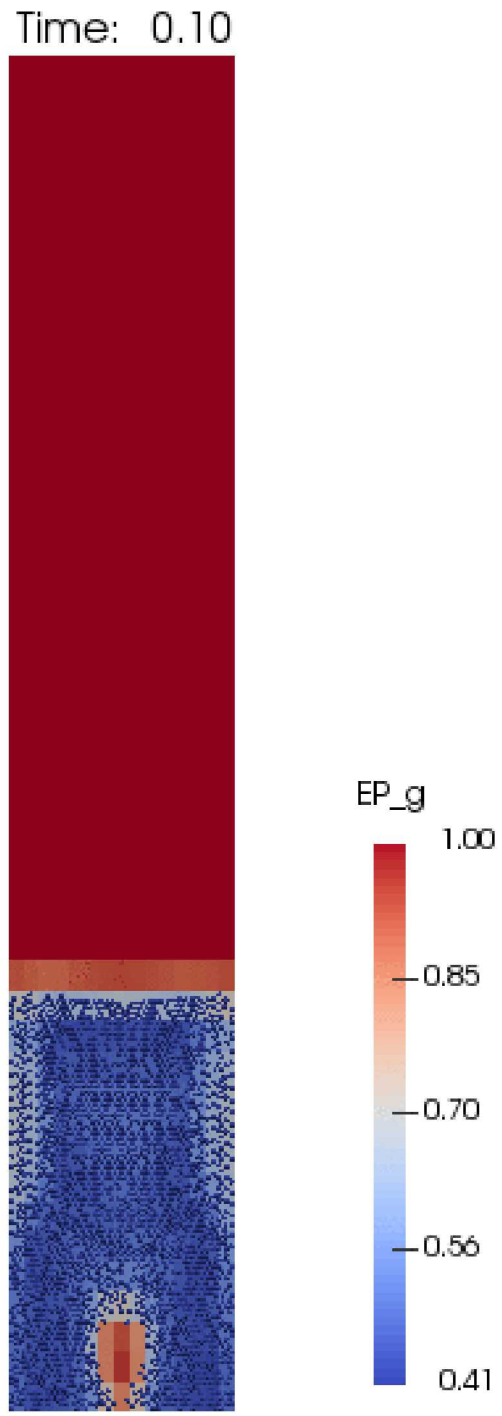
Flow in the fluidized bed

- Central jet fluidized bed using DEM simulations.
- The air is injected at a speed of 4200 cm/s through a narrow inlet having width of 1 cm and located exactly at the geometric center of the bottom wall.
- The air exits to atmospheric conditions at the top. No-slip boundary conditions are specified for the gas-phase velocity at the walls.
- cells having width of 1 cm and height of 2 cm, resulting in a total of 675 (=15x45) computational cells.
- The bed is initialized with 217.15 g of particles with a diameter of 0.4 cm and density of 2.7 g/cm3, resulting in total of 2400 spherical particles.

Average bed height = 14.3808 cm



parameter	value
Particle-particle restitution co-efficient	0.80
Particle-wall restitution co-efficient	0.80



Dakota-MFiX results: Flow in a fluidized bed

Input 1 - $e_{p,n}$	Input 2 - $e_{w,n}$
N(0.8,0.04)	N(0.8,0.04)

$e_{p,n}$ = particle-particle restitution co-efficient

$e_{w,n}$ = particle-wall restitution co-efficient

Response function
Bed height = $\sum_{n=1}^{N_p} Y^n / N_p$

N_p = Number of particles (=2400)

Y = y- coordinate of n^{th} particle's position at time t

	PCE, Order =5 sample size =25	LHS, sample size =500
Mean	14.4081	14.4171
Std	3.6230e-02	3.4146e-02

Partial Correlation Matrix between input and output:

	response_fn_1
x1	5.0089e-01
x2	-2.2879e-01

Dakota-MFiX results: Flow in a fluidized bed

Normal distribution, LHS, # of uncertain input variables = 9

	D_p (cm)	U_{inlet} (cm/s)	$e_{p,n}$	$e_{w,n}$	KN (g/s^2)	KN_W (g/s^2)	MEW	MEW_W	μ_g (g/ cm s)
mean	0.34	4200	0.8	0.8	1000000	1000000	0.1	0.1	0.00018
std	0.0297	367.5	0.07	0.07	87500	87500	0.0087	0.0087	0.00001575

D_p = Particle diameter
U_{inlet} = Velocity of the fluidizing agent at the inlet
$e_{p,n}$ = particle-particle restitution co-efficient
$e_{w,n}$ = particle-wall restitution co-efficient
KN = Particle – particle normal collision spring constant
KN_W = Particle – wall normal collision spring constant
MEW = Particle - particle friction co-efficient
MEW_W = particle – wall friction co-efficient
μ_g = Viscosity of the fluidizing agent at the inlet

Response function

1. Average bed height $H_p(t) = \sum_{n=1}^{N_p} Y^n / N_p$

2. Maximum pressure difference across the bed

Dakota-MFiX results: Flow in a fluidized bed

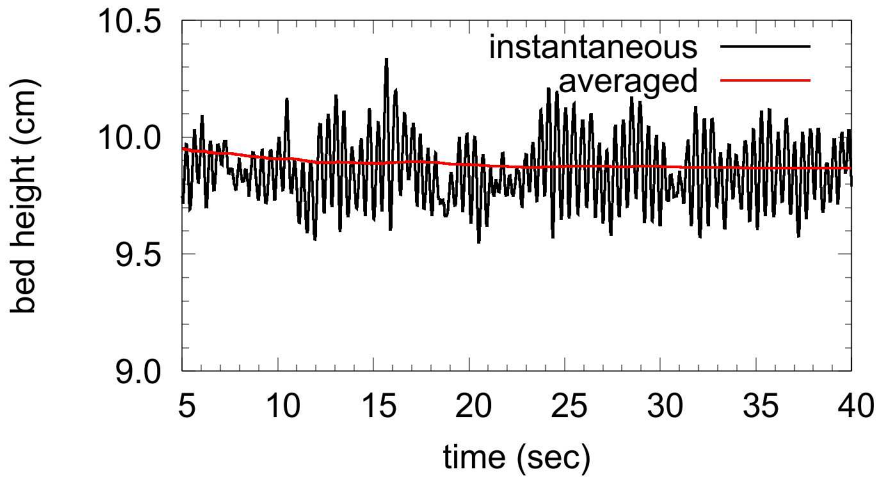
of uncertain input variables = 9

	D_p (cm)	U_{inlet} (cm/s)	$e_{p,n}$	$e_{w,n}$	KN (g/s^2)	KN_W (g/s^2)	MEW	MEW_W	μ_g (g/ cm s)
mean	0.34	4200	0.8	0.8	1000000	1000000	0.1	0.1	0.00018

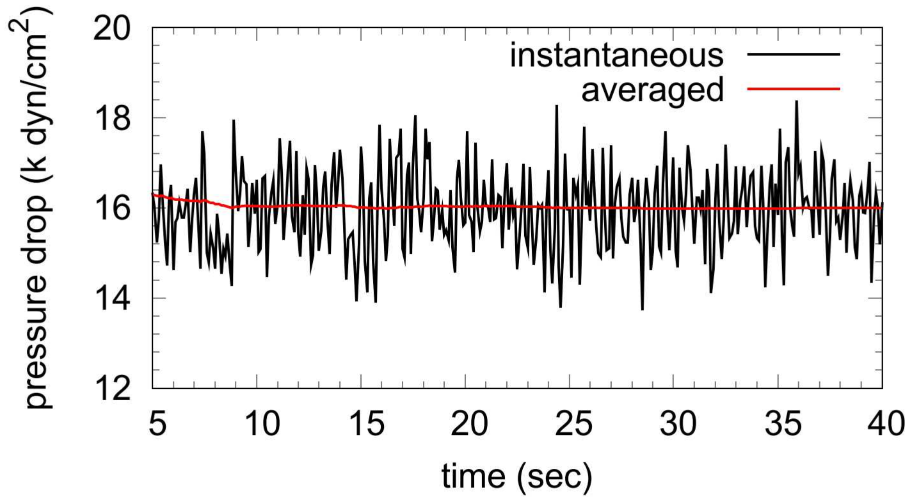
Response function

1. Average bed height $H_p(t) = \sum_{n=1}^{N_p} Y^n / N_p$

2. Maximum pressure difference across the bed



Bed height at t=40 is 9.868 cm



Max pressure difference at t=40 is 15.991 k dn/cm^2

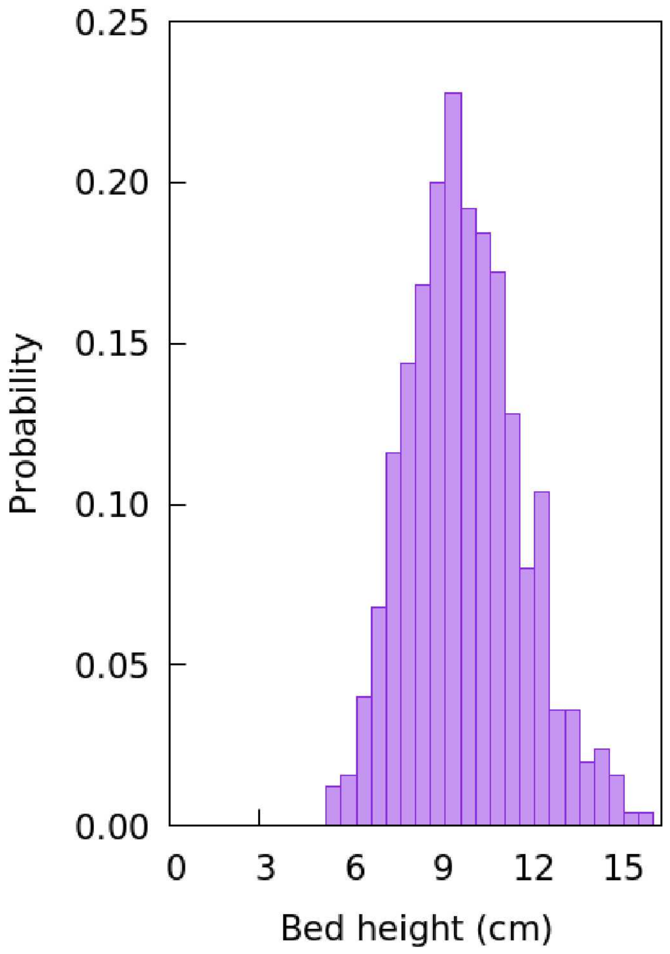
Response function – bed height

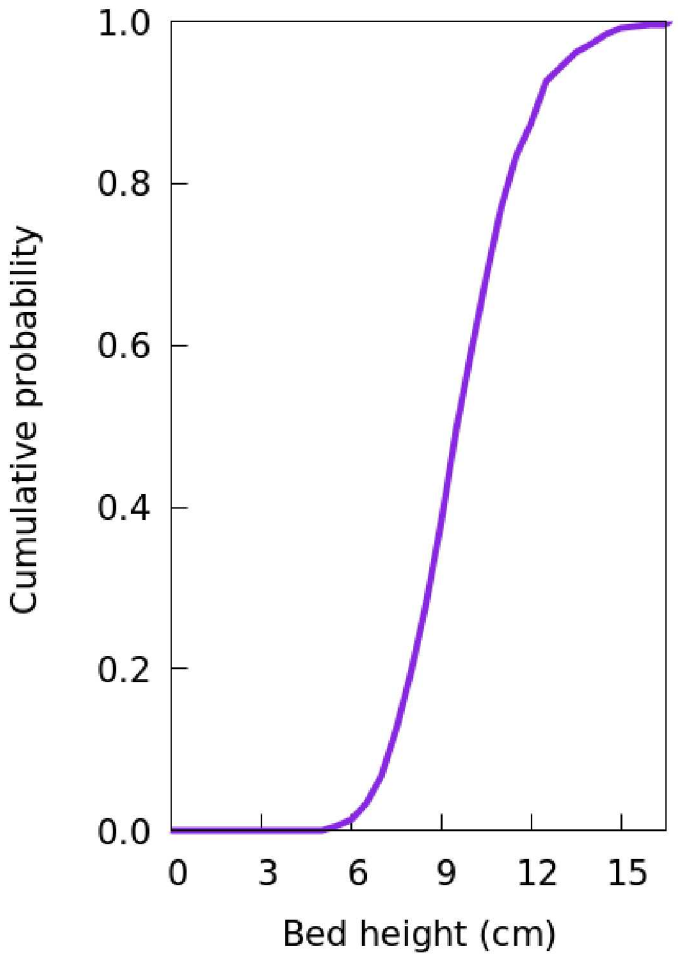
Normal distribution, LHS, sample size = 500

Mean: 9.6827
Std: 1.9529

Partial Correlation Matrix between input and output:

	Bed height
D_p	9.87853e-01
U_{inlet}	7.65915e-01
$e_{p,n}$	1.26841e-03
$e_{w,n}$	-2.19558e-02
KN	-5.44667e-02
KN_W	-4.08984e-02
MEW	-1.03671e-02
MEW_W	6.74702e-02
μ_g	-1.76986e-02





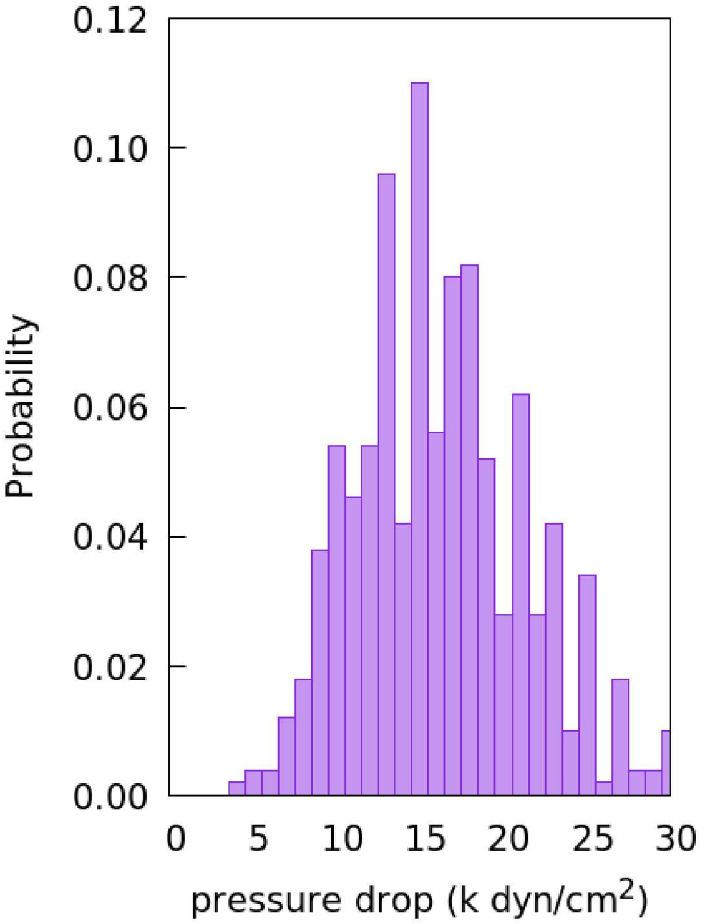
Response function – Max pressure difference across the bed

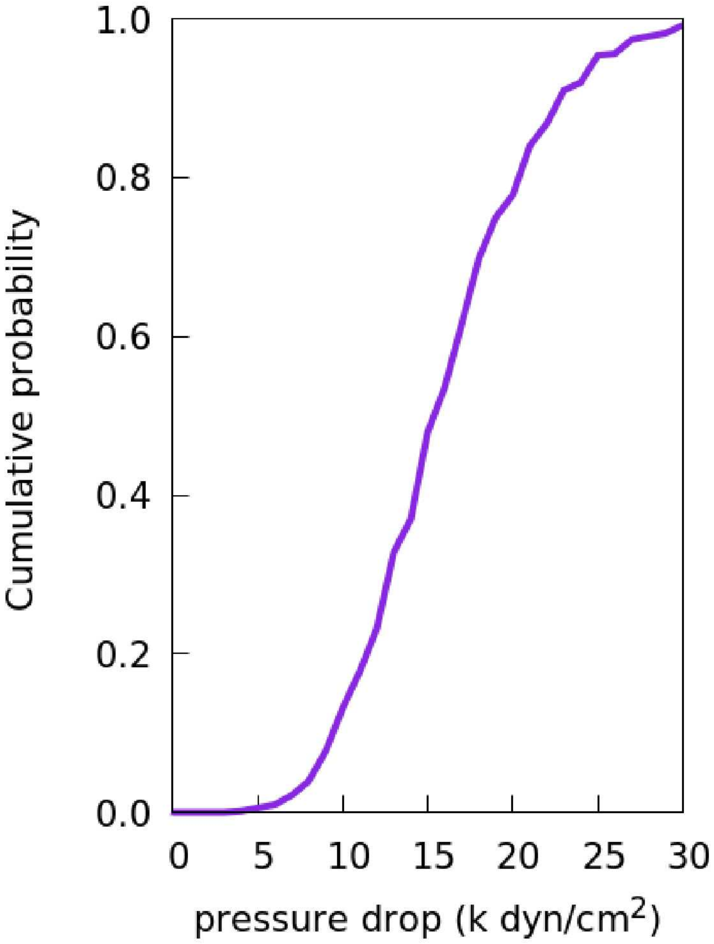
Normal distribution, LHS, sample size = 500

Mean:	1.5857e+04
Std:	5.2590e+03

Partial Correlation Matrix between input and output:

	Pressure drop
D_p	9.81640e-01
U_{inlet}	-4.91593e-01
$e_{p,n}$	5.73839e-02
$e_{w,n}$	1.11189e-01
KN	-7.00940e-02
KN_W	-1.14437e-02
MEW	3.87739e-02
MEW_W	3.50937e-02
μ_g	-2.23406e-02





Acknowledgement

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XSEDE Extreme Science and Engineering Discovery Environment
TACC Texas Advanced Computing Center
SDSC San Diego Supercomputer Center
BRIDGES A Pittsburgh Supercomputing Center Resource
Research Cloud @UTEP Accelerating Discovery

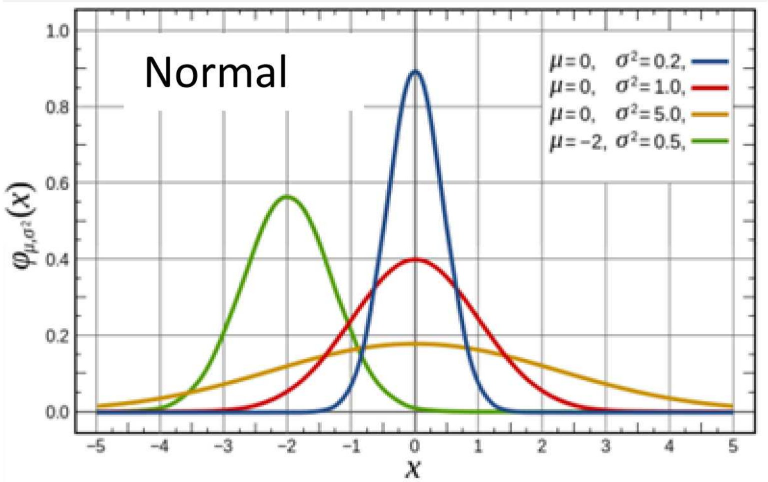
Thank you

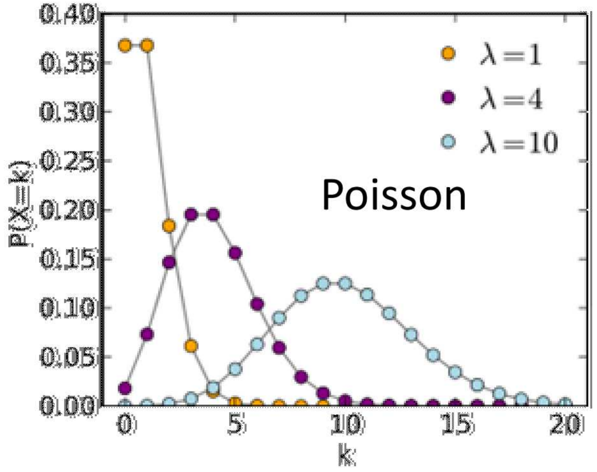
Thank you

Characterizing Uncertainties to Dakota

Must characterize each variable's uncertainty and (optionally) any correlation between pairs of variables. Need not be normal (or uniform)!

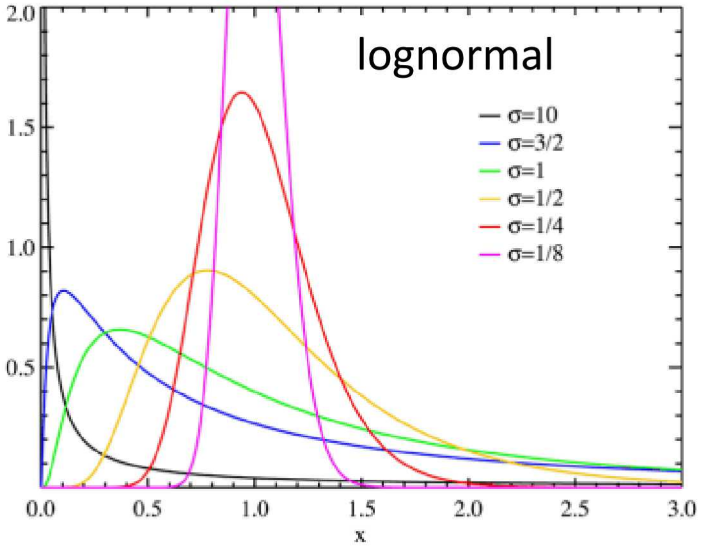
- May require processing data with math/stats tool to fit distributions, performing literature searches, or querying experts

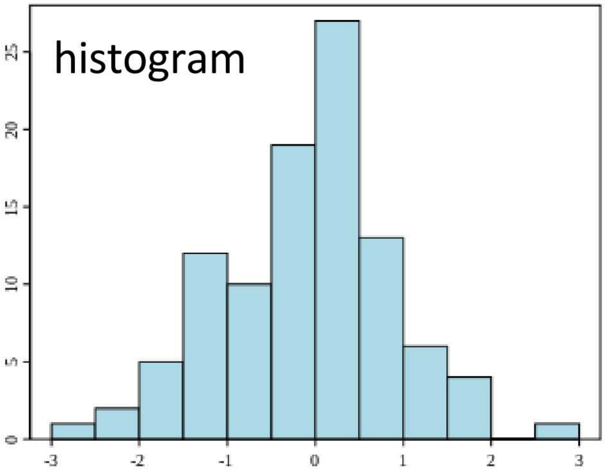




Dakota uncertain variable types:

- Aleatory continuous: **normal**, lognormal, uniform, loguniform, triangular, exponential, beta, gamma, Gumbel, Frechet, Weibull, histogram
- Aleatory discrete: Poisson, binomial, negative binomial, hypergeometric, histogram point
  Epistemic: continuous interval, discrete interval, discrete set





Response function – bed height

Normal distribution

	LHS, sample size = 500	gaussian_process surfpack	Global nueral network	Global mars
Mean:	9.6826836828e+00	9.6850171779e+00	9.6762857192e+00	9.6835642134e+00
Std:	1.9528769373e+00	1.9410264354e+00	1.9423379855e+00	1.9448349902e+00

-0.112585 + 0.990706*x0 + 0.189103*x1 +
0.00483635*x2 -0.00142171*x3 -
0.00356067*x4 + 0.000614168*x5 -
0.00888153*x6 + 0.00596127*x7
0.00369133*x8 + 0.491255*x0^2 -
0.0590336*x1^2 + 0.0806555*x2^2 -
0.00036364*x3^2 - 0.0214853*x4^2 -
0.00213713*x5^2 -0.0434566*x6^2 +
0.0396718*x7^2 + 0.0211821*x8^2

9.6816878179e+00
1.9446660490e+00