Guidance to reviewers

SAND2016-6201PE

- These CASL VERA / COBRA-TF examples will supplement the standard Dakota Software Training materials:
  - SAND2015-6794TR (Overview)
  - SAND2016-3330PE (SA)
  - SAND2016-1198PE (UQ)
  - SAND2015-6869TR (Input Components)
  - SAND2015-6867TR (Interfacing)
- Only the new VERA/application-specific content is submitted in this review
- The examples are based on a single rod COBRA-TF thermal-hydraulics analysis extracted from the open source COBRA-TF test suite.

Compilation of SAND2015-6794TR (Overview), SAND2016-3330PE (SA), SAND2016-1198PE (UQ), SAND2015-6869TR (Input Components), SAND2015-6867TR (Interfacing), with new CASL-specific exercise/demo problems SAND2016-XXXXYY

Sensitivity and Uncertainty Analysis with VERA's Dakota Module

Brian Adams and Russell Hooper

Sandia National Laboratories

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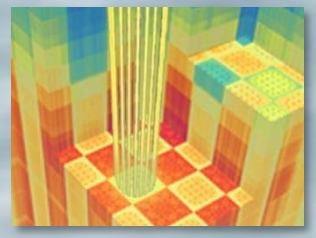
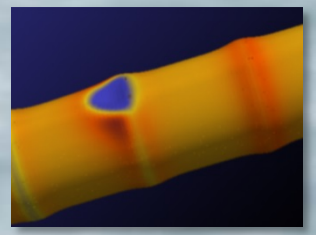
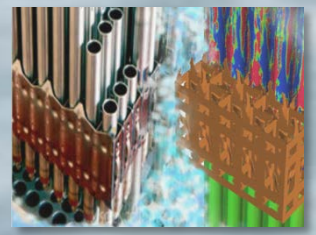
Consortium for Advanced Simulation of Light-Water Reactors (CASL) Summer Institute 2016

June 21 – July 1, 2016

Oakridge, TN







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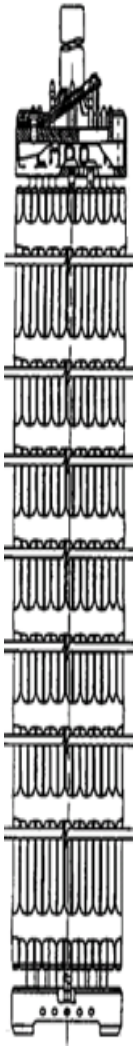
Sensitivity and Uncertainty Analysis with VERA's Dakota Module

Sandia National Laboratories

- Sensitivity Analysis (SA)
  - What is SA? Why should you care? How do you do it?
  - Explore some SA problems with Dakota and VERA
  - Understand methods for performing SA: parameter studies and sampling
- Dakota capability overview
- Uncertainty Quantification (UQ)
  - What is UQ? Why should you care? How do you do it?
  - Explore some UQ problems with Dakota and VERA
  - Understand methods for performing UQ: sampling, reliability, and polynomial chaos
- Dakota interface to VERA

Discussion:
Sensitivity Analysis for VERA Simulations



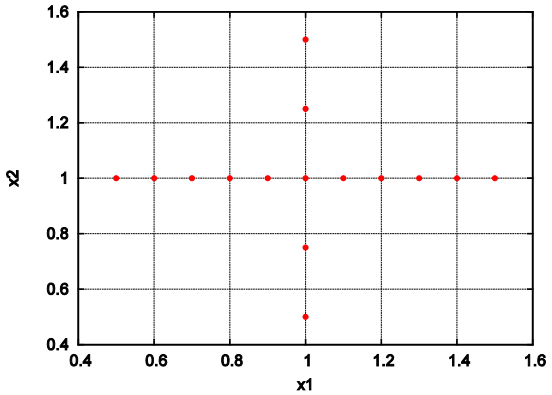
Consider the COBRA-TF simulations presented earlier in the Institute

- What is an example simulation output of interest (quantity of interest)?
- What kinds of parameters in the VERA input might/might not affect it? What about factors not in VERA input?
- How might you determine which parameters are the most influential on the QoI? What challenges might you face in assessing this?
- How might your answers change if the simulator changes, e.g., coupled physics? Or the end analysis goal changes? If your computational budget is limited?

Specifying Dakota Variable Ranges for a Sensitivity Study

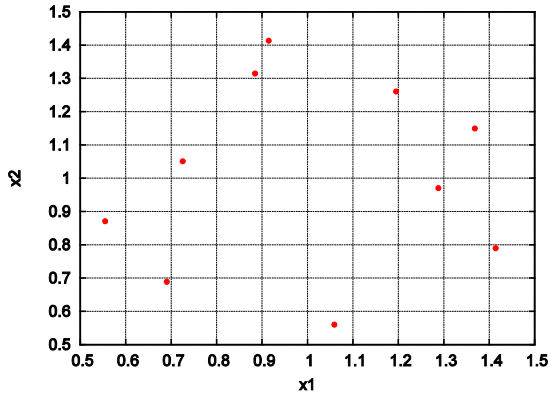
Local or univariate global sensitivity: initial point and steps to take

```
variables
  continuous_design  2
    descriptors      '*CORE/rated_flow'
                     '*COBRATF/hgap'
    initial_point     1.0    1.0

method centered_parameter_study
  steps_per_variable  5      2
  step_vector         0.1    0.25
```



Global sensitivity: hyper-rectangle bounds

```
variables
  continuous_design  2
    descriptors      '*CORE/rated_flow'
                     '*COBRATF/hgap'
    initial_point     1.0      1.0
    lower_bounds      0.95     0.9
    upper_bounds      1.05     1.1

method sampling  ...
```



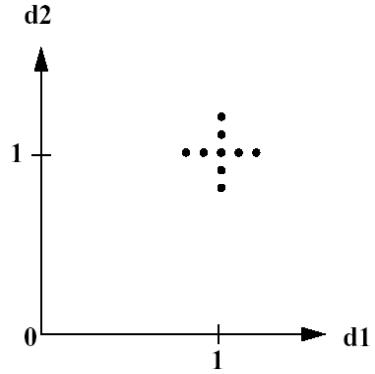
Dakota variable type is not critical. Typically use continuous or discrete design, or uniform or discrete (interval, set) uncertain.

Exercise 1: Centered Parameter Study for Univariate Sensitivity

- Begin by manually perturbing a parameter, e.g., COBRA's hgap, and observing the effects on the QoIs, such as pressure drop, max fuel temperature, and max pin power

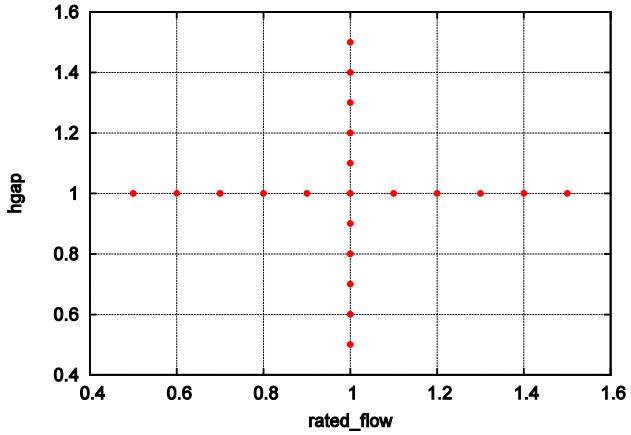
  change parameters $\pm 5\%, \pm 10\%$, etc.

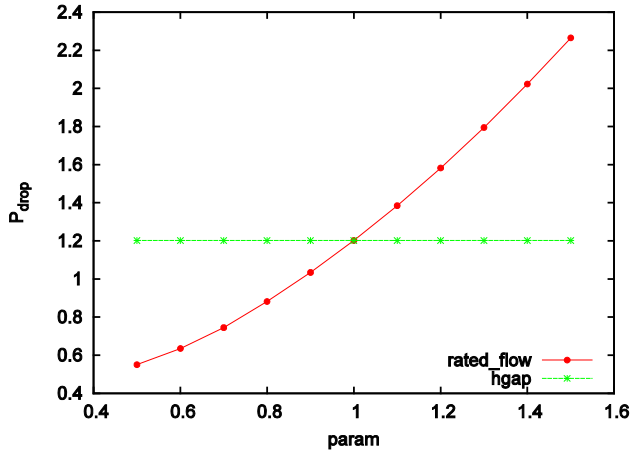
- Automate this approach using Dakota to drive a CPS
  (a Dakota input file is provided in your course materials)
- Requires $(2 \times d \times steps + 1)$ runs
- How do we interpret this study for SA purposes?
  - Overall range of variability
  - Nonlinear effects
  - Relative influence
  - (Helps to plot the tabular data overlaid to compare)

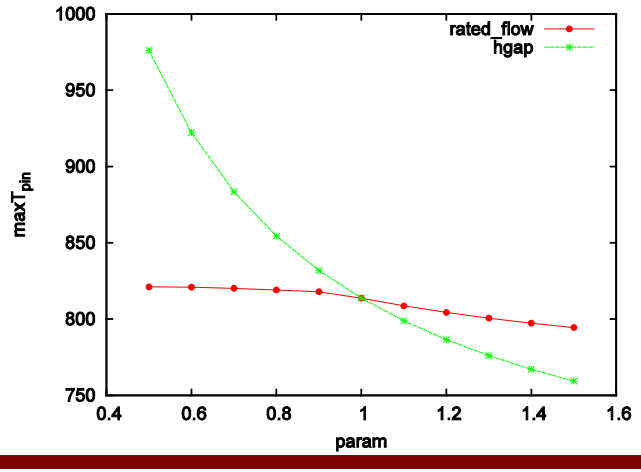


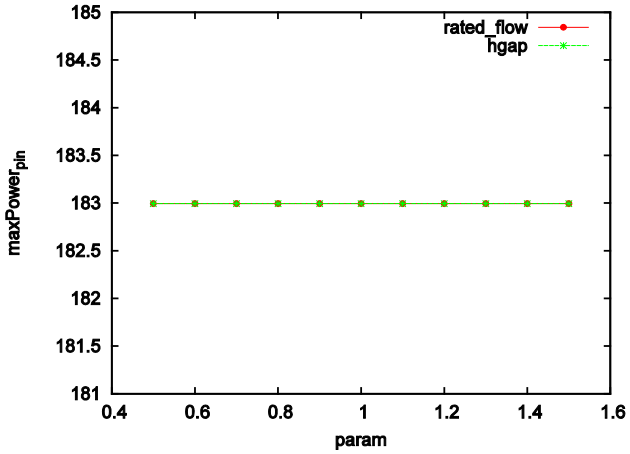
Exercise 1: CPS Results

- A CPS is helpful for quick screening, characterizing a model
- What would you conclude from these output plots?



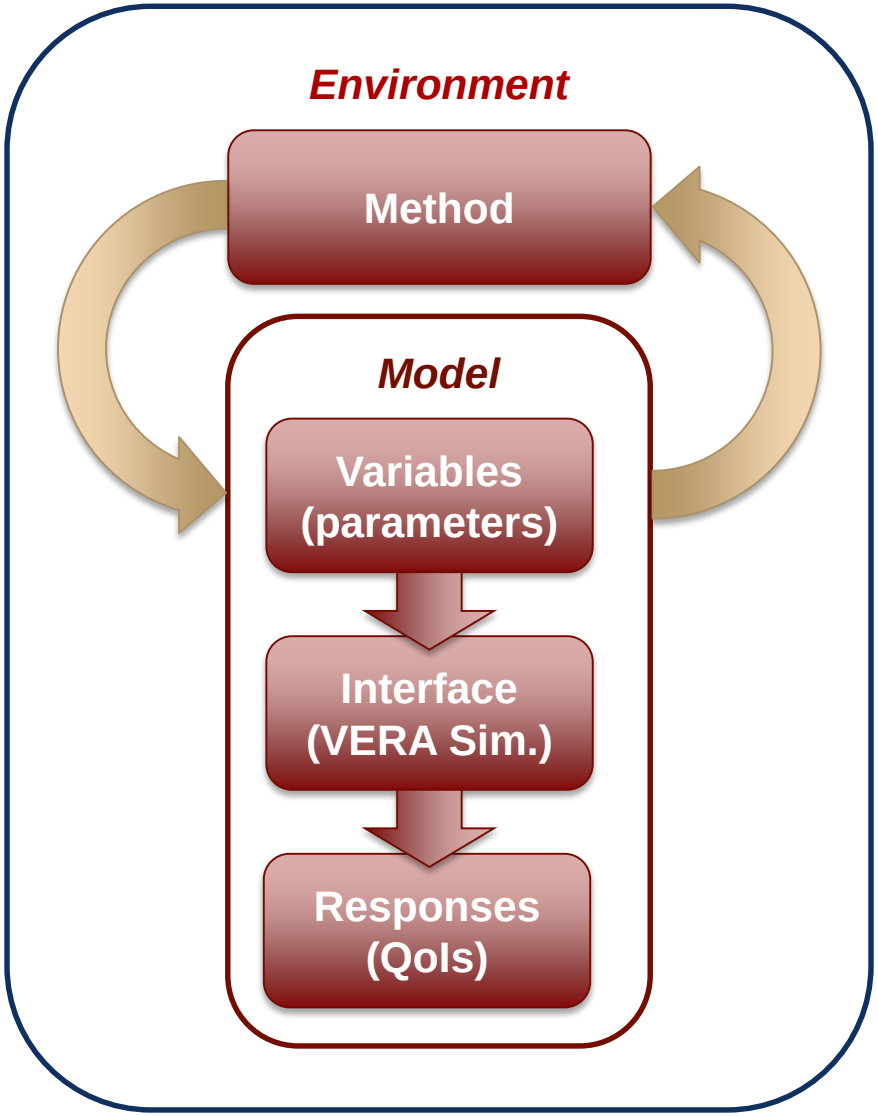






Dakota Input

```
environment
    tabular_data output_precision 1e-16

method
  centered_parameter_study
    step_vector         0.1  0.1
    steps_per_variable  5    5

model
  single

variables
  active all
  continuous_design = 2
    initial_point       1.0  1.0
    descriptors        '*CORE/rated_flow‘
                       '*COBRATF/hgap'

interface
  fork
    analysis_drivers = ‘dakota-vera-analysis.sh'

responses
  response_functions = 3
    descriptors = 'TotalPressure'
                  'MaxPinTemp'
                  'MaxPinPower'
  no_gradients
  no_hessians
```



Dakota to VERA Adapter

vera.inp

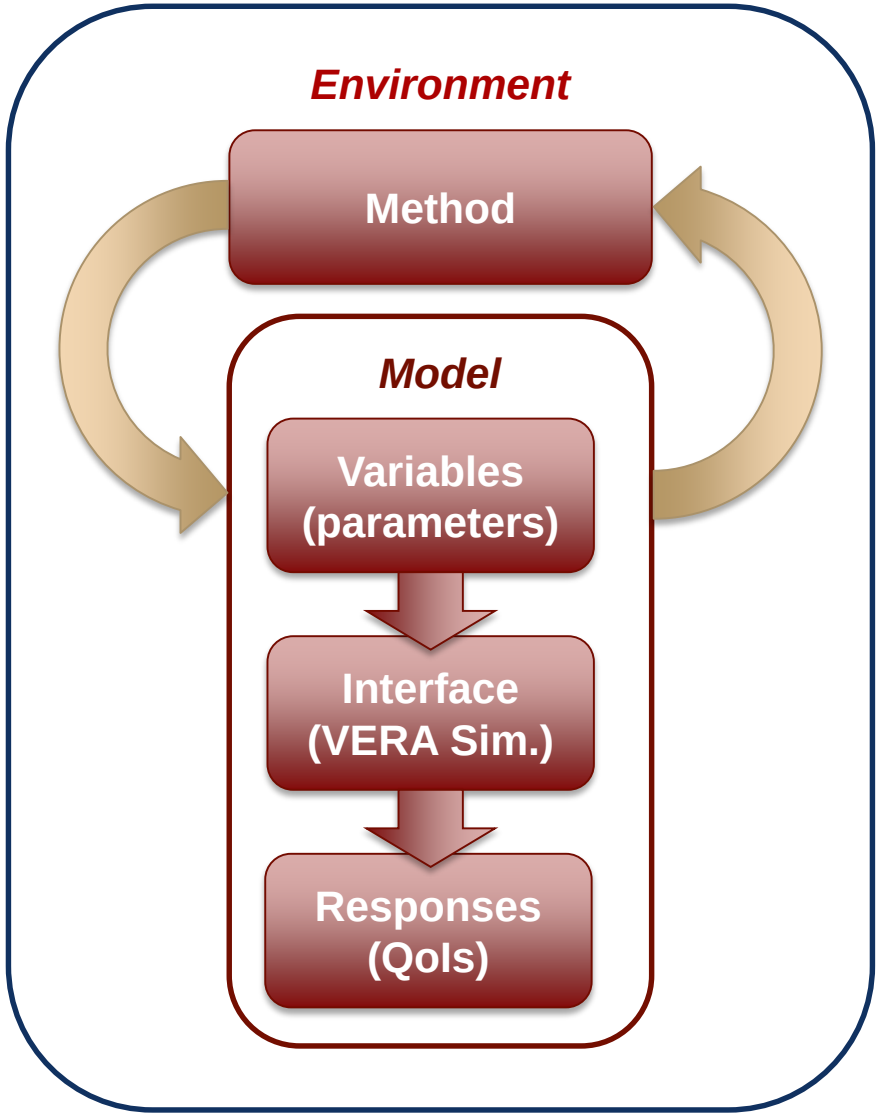
VERAInExt/verain/scripts/react2xml.pl

```
# vera.xml
<ParameterList name="COBRATF">
  ...
  <Parameter name="hgap" type="double"
   value="5678.3" />
 ...
</ParameterList>
```

DakotaVERAIn.py

```
*COBRATF/hgap = 1.1
```

```
# vera.xml
<ParameterList name="COBRATF">
 ...
  <Parameter name="hgap" type="double"
   value="6246.13" />
  ...
</ParameterList>
```



Exercise 2: Random Sampling for SA

- Use the Reference Manual to change the Dakota input file in **`dakota_cps_study.in`** from a centered study to sampling
  - Configure the sampling method to perform a Latin hypercube sample with an appropriate number of samples. Why might a **`seed`** specification be important?
  - Use **`uniform_uncertain`** variables to define the hyper-rectangle given by
    $0.5 \leq$ *CORE/rated_flow ≤ 1.5 $0.5 \leq$ *COBRATF/hgap ≤ 1.5

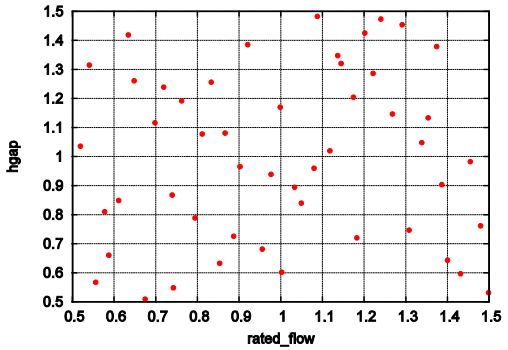
- Run the study and examine the correlations between inputs and outputs
  - Which parameters most influence each quantity of interest?
  - How does changing the number of samples affect your conclusions?
  - Do these match your intuition of channel flow behavior?

Exercise 2 Results: Global Sampling for COBRA-TF

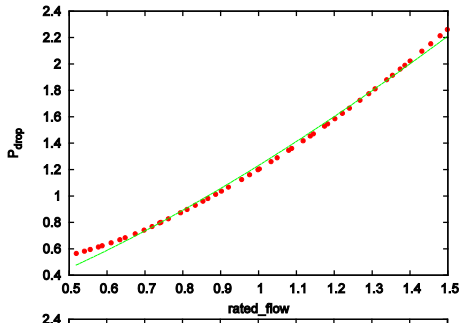
Partial Correlation Matrix for CTF

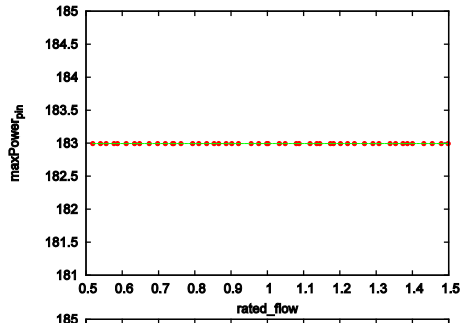
	TotalPressure	MaxPinTemp	MaxPinPower
*CORE/rated_flow	9.93E-01	-4.71E-01	0.00E+00
*COBRATF/hgap	-2.17E-01	-9.62E-01	0.00E+00

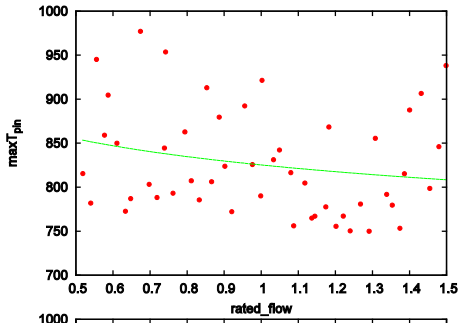
partial correlations from console output (colored w/ Excel)

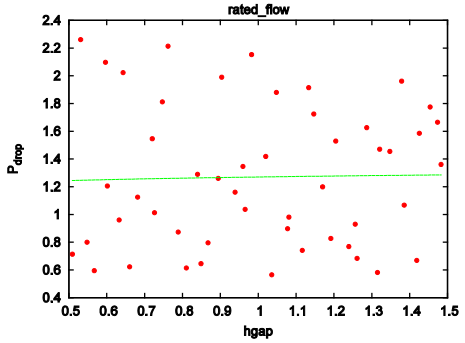


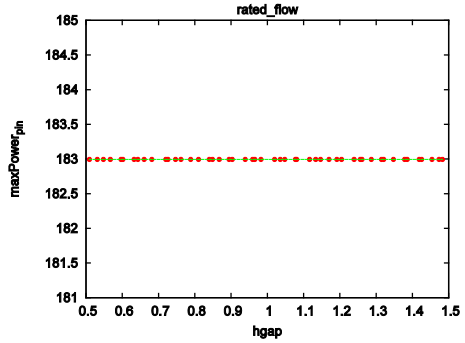
Scatter plots: Dakota tabular data plotted in GNUPlot (can use Minitab, Matlab, JMP, Excel, …)

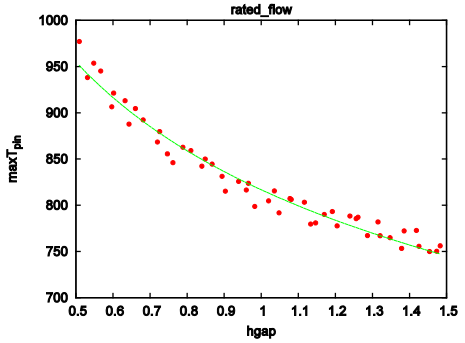












Discussion:
Uncertainties in NE Simulations

Generally,

- Name some key uncertainties that affect nuclear engineering experiments, analysis, and work products.
- What factors might account for discrepancies between modeling/simulation and reality?
- What simulation input data are you confident in? Less sure of?
- What do decision makers expect: a number out of the code, a range of possibilities, something else?

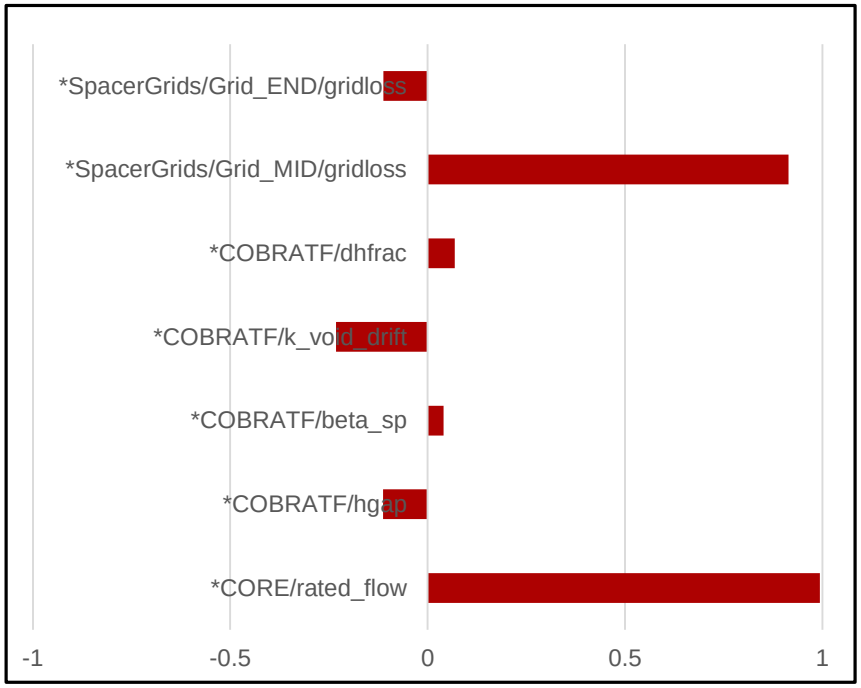
Specifically, for the COBRA-TF simulations discussed earlier, consider the most influential input parameters from SA:

- Do they take on a single value or a distributions?
- How might you characterize their uncertainty?
- How might you assess the resulting output (prediction) variability?

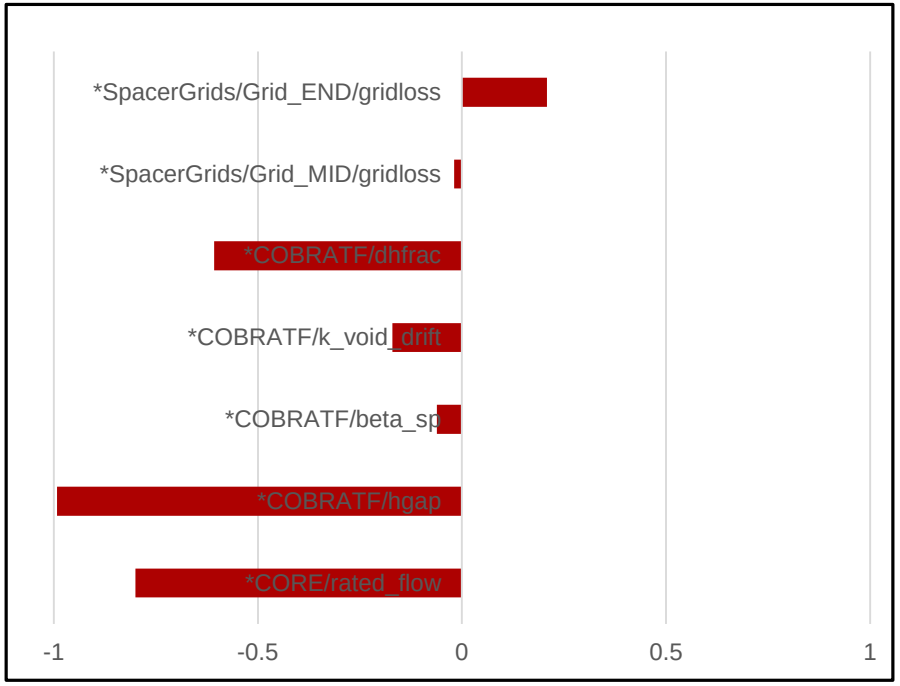
Exercise 1: Sampling-based UQ

Given the following partial correlation results from a previous LHS sampling study with COBRA-TF…

Total Pressure Drop



Max Pin Temp



Exercise 1: Sampling-based UQ

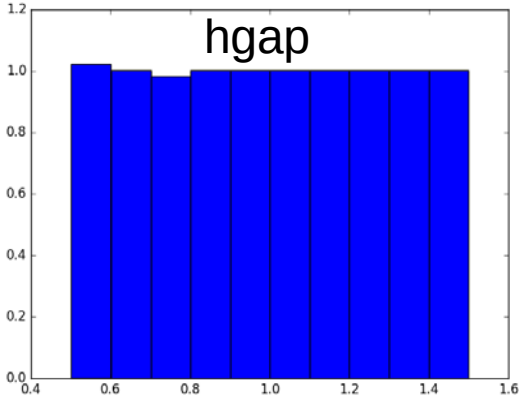
- Down-select: Choose a QoI and determine which parameters to include in a UQ study
- Characterize: Using resources, potentially including expert opinion, choose distributions to describe parameter uncertainty, i.e., bounds, variation, distribution function
- Forward UQ: Modify the LHS Dakota sampling study to perform a forward UQ study using the down-selected parameters and their uncertainty characterizations
- Answer the following:
  - What is the QoI mean and variance or (standard deviation)?
  - What is the probability of the QoI exceeding an important threshold value (specifically, 2.5atm for Total Pressure Drop and 950deg for Max Pin Temp)? *Hint: you may need the `response_levels` keyword.*

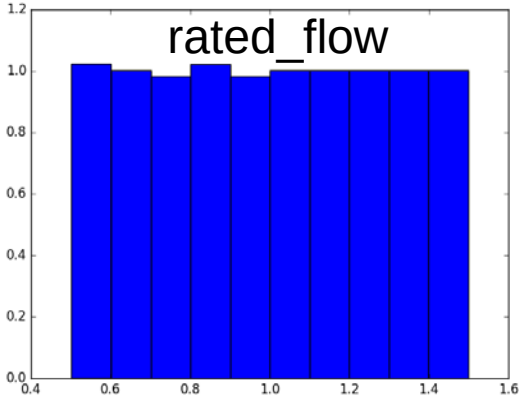
Exercise Questions

- Where do you find the relevant Dakota output?
- What statistical quantities do you find in the output?

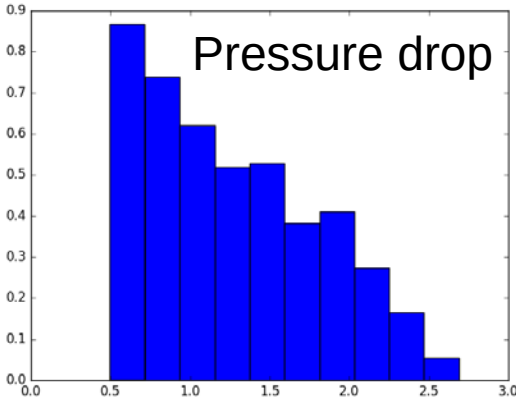
- Extra 1: What happens if you increase/decrease the number of samples?
- Extra 2: What happens if you change the uncertainty characterization of one or more variables?

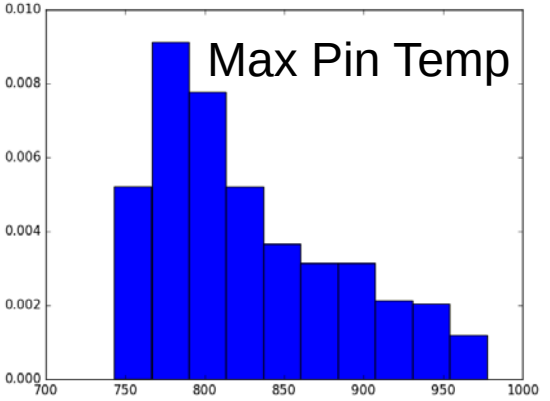
Observations: PDFs





"My variables are uniformly distributed. Doesn't that mean that my responses will be, too?"





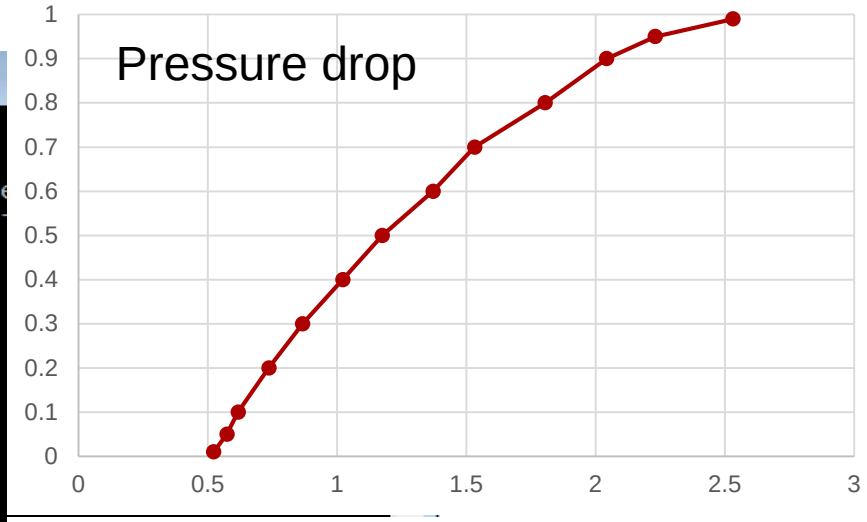
Standardized probability plots (not shown) can show how well the Dakota-generated sample data follow an assumed distribution

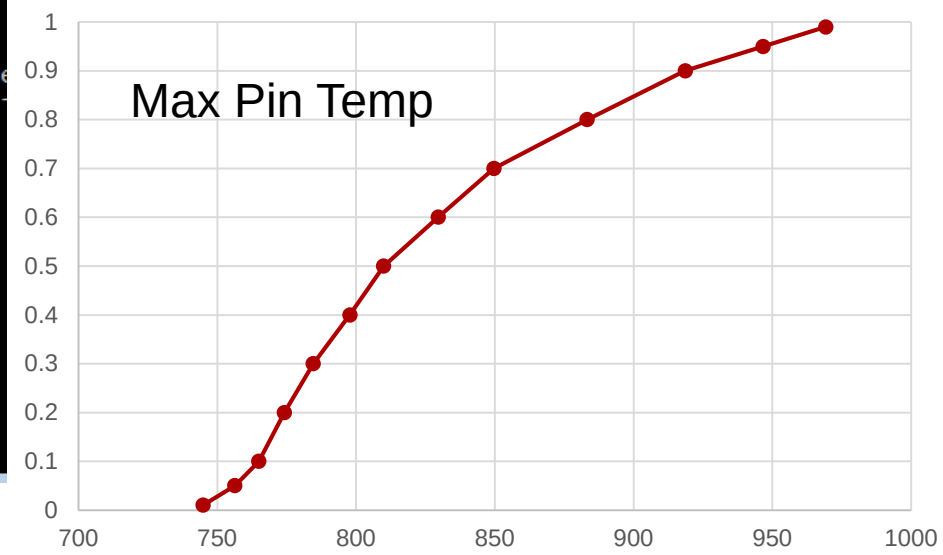
Exercise Solutions

```
<<<<< Function evaluation summary: 500 total (500 new, 0 duplicate)
------------------------------------------------------------------------------
Statistics based on 500 samples:

Sample moment statistics for each response function:
                            Mean           Std Dev          Skewness          Kurtosis
 TotalPressure  1.2684274200e+00  5.3632857704e-01  5.0472688719e-01 -7.5527300880e-01
    MaxPinTemp  8.2706575765e+02  5.8430203973e+01  7.3763812152e-01 -4.5303266907e-01

95% confidence intervals for each response function:
                  LowerCI_Mean      UpperCI_Mean    LowerCI_StdDev    UpperCI_StdDev
 TotalPressure  1.2213027114e+00  1.3155521286e+00  5.0501958333e-01  5.7180760725e-01
    MaxPinTemp  8.2193176619e+02  8.3219974912e+02  5.5019252240e+01  6.2295459453e+01

Probability Density Function (PDF) histograms for each response function:
PDF for TotalPressure:
          Bin Lower          Bin Upper      Density Value
          ---------          ---------      -------------
   4.9627000000e-01   5.2273000000e-01   3.7792894936e-01
   5.2273000000e-01   5.7384000000e-01   7.8262570925e-01
   5.7384000000e-01   6.1727000000e-01   1.1512779185e+00
   6.1727000000e-01   7.3623000000e-01   8.4061869536e-01
   7.3623000000e-01   8.6682000000e-01   7.6575541772e-01
   8.6682000000e-01   1.0222300000e+00   6.4345923686e-01
   1.0222300000e+00   1.1752000000e+00   6.5372295221e-01
   1.1752000000e+00   1.3709900000e+00   5.1075131518e-01
   1.3709900000e+00   1.5320000000e+00   6.2107943606e-01
   1.5320000000e+00   1.8052900000e+00   3.6591166892e-01
   1.8052900000e+00   2.0425500000e+00   4.2147854674e-01
   2.0425500000e+00   2.2309300000e+00   2.6542095764e-01
   2.2309300000e+00   2.5000000000e+00   1.4122718995e-01
   2.5000000000e+00   2.5316400000e+00   6.3211125158e-02
   2.5316400000e+00   2.6893900000e+00   6.3391442155e-02
PDF for MaxPinTemp:
          Bin Lower          Bin Upper      Density Value
          ---------          ---------      -------------
   7.4308235613e+02   7.4481769604e+02   5.7625598073e-03
   7.4481769604e+02   7.5625161052e+02   3.4983644533e-03
   7.5625161052e+02   7.6494343717e+02   5.7525307450e-03
   7.6494343717e+02   7.7413659558e+02   1.0877654392e-02
   7.7413659558e+02   7.8451031069e+02   9.6397480469e-03
   7.8451031069e+02   7.9770714446e+02   7.5775751812e-03
   7.9770714446e+02   8.0987656943e+02   8.2173151345e-03
   8.0987656943e+02   8.2953675049e+02   5.0864231451e-03
   8.2953675049e+02   8.4968444855e+02   4.9633461697e-03
   8.4968444855e+02   8.8320763820e+02   2.9830097037e-03
   8.8320763820e+02   9.1855688305e+02   2.8289147451e-03
   9.1855688305e+02   9.4661545726e+02   1.7819864840e-03
   9.4661545726e+02   9.5000000000e+02   3.5455306428e-03
   9.5000000000e+02   9.6919264513e+02   1.4588921858e-03
   9.6919264513e+02   9.7758288088e+02   1.1918616232e-03
                                                  12095,4       99%
```

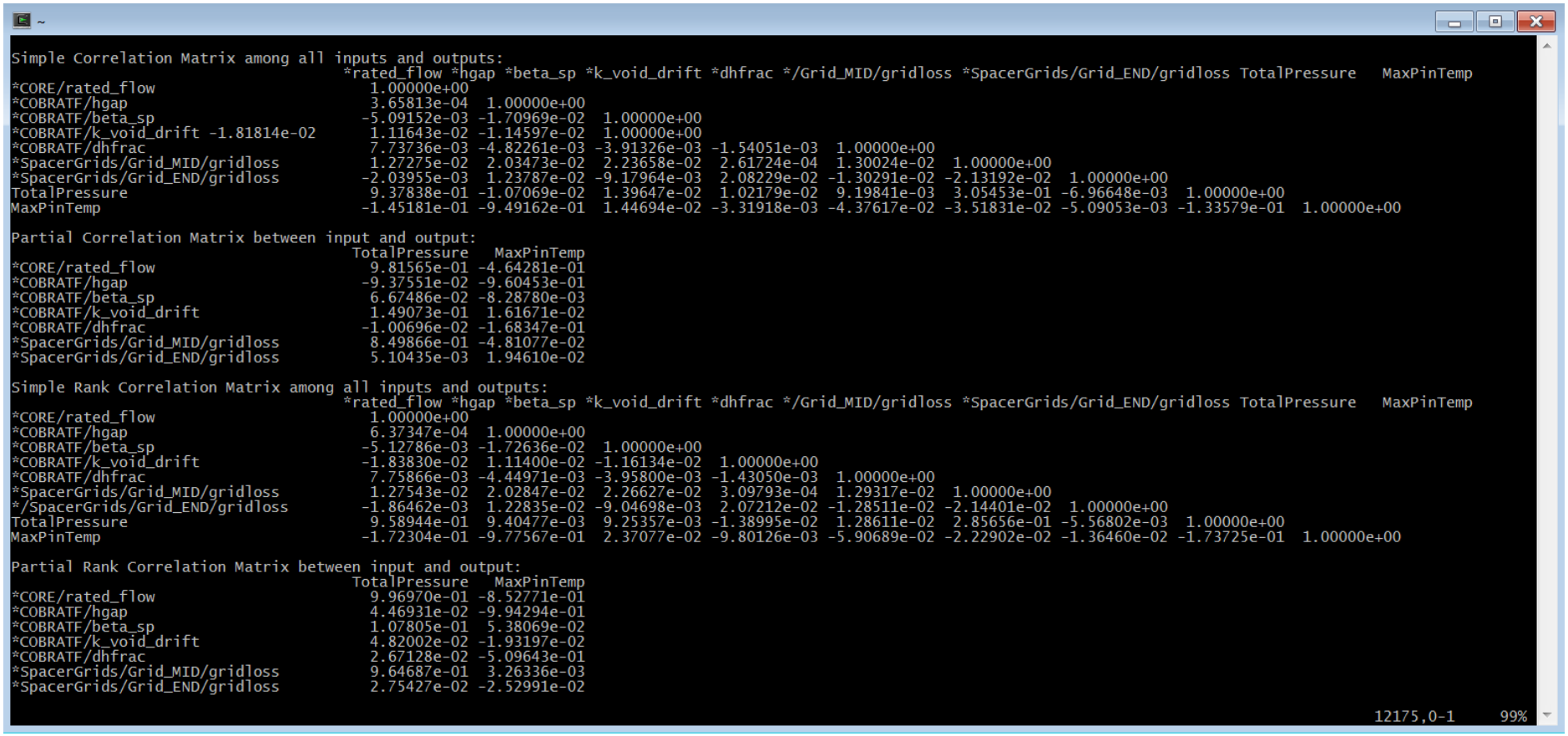
Exercise Solutions

```
~

Level mappings for each response function:
Cumulative Distribution Function (CDF) for TotalPressure:
     Response Level  Probability Level  Reliability Index  Ge
     --------------  -----------------  -----------------  --
   2.5000000000e+00   9.8800000000e-01
   5.2273000000e-01   1.0000000000e-02
   5.7384000000e-01   5.0000000000e-02
   6.1727000000e-01   1.0000000000e-01
   7.3623000000e-01   2.0000000000e-01
   8.6682000000e-01   3.0000000000e-01
   1.0222300000e+00   4.0000000000e-01
   1.1752000000e+00   5.0000000000e-01
   1.3709900000e+00   6.0000000000e-01
   1.5320000000e+00   7.0000000000e-01
   1.8052900000e+00   8.0000000000e-01
   2.0425500000e+00   9.0000000000e-01
   2.2309300000e+00   9.5000000000e-01
   2.5316400000e+00   9.9000000000e-01
Cumulative Distribution Function (CDF) for MaxPinTemp:
     Response Level  Probability Level  Reliability Index  Ge
     --------------  -----------------  -----------------  --
   9.5000000000e+02   9.6200000000e-01
   7.4481769604e+02   1.0000000000e-02
   7.5625161052e+02   5.0000000000e-02
   7.6494343717e+02   1.0000000000e-01
   7.7413659558e+02   2.0000000000e-01
   7.8451031069e+02   3.0000000000e-01
   7.9770714446e+02   4.0000000000e-01
   8.0987656943e+02   5.0000000000e-01
   8.2953675049e+02   6.0000000000e-01
   8.4968444855e+02   7.0000000000e-01
   8.8320763820e+02   8.0000000000e-01
   9.1855688305e+02   9.0000000000e-01
   9.4661545726e+02   9.5000000000e-01
   9.6919264513e+02   9.9000000000e-01
```





Exercise Solutions



```
~

Simple Correlation Matrix among all inputs and outputs:
                          *rated_flow *hgap *beta_sp *k_void_drift *dhfrac */Grid_MID/gridloss *SpacerGrids/Grid_END/gridloss TotalPressure   MaxPinTemp
*CORE/rated_flow            1.00000e+00
*COBRATF/hgap               3.65813e-04  1.00000e+00
*COBRATF/beta_sp           -5.09152e-03 -1.70969e-02  1.00000e+00
*COBRATF/k_void_drift -1.81814e-02      1.11643e-02 -1.14597e-02  1.00000e+00
*COBRATF/dhfrac             7.73736e-03 -4.82261e-03 -3.91326e-03 -1.54051e-03  1.00000e+00
*SpacerGrids/Grid_MID/gridloss          1.27275e-02  2.03473e-02  2.23658e-02  2.61724e-04  1.30024e-02  1.00000e+00
*SpacerGrids/Grid_END/gridloss         -2.03955e-03  1.23787e-02 -9.17964e-03  2.08229e-02 -1.30291e-02 -2.13192e-02  1.00000e+00
TotalPressure               9.37838e-01 -1.07069e-02  1.39647e-02  1.02179e-02  9.19841e-03  3.05453e-01 -6.96648e-03  1.00000e+00
MaxPinTemp                 -1.45181e-01 -9.49162e-01  1.44694e-02 -3.31918e-03 -4.37617e-02 -3.51831e-02 -5.09053e-03 -1.33579e-01  1.00000e+00

Partial Correlation Matrix between input and output:
                          TotalPressure   MaxPinTemp
*CORE/rated_flow            9.81565e-01 -4.64281e-01
*COBRATF/hgap              -9.37551e-02 -9.60453e-01
*COBRATF/beta_sp            6.67486e-02 -8.28780e-03
*COBRATF/k_void_drift       1.49073e-01  1.61671e-02
*COBRATF/dhfrac            -1.00696e-02 -1.68347e-01
*SpacerGrids/Grid_MID/gridloss          8.49866e-01 -4.81077e-02
*SpacerGrids/Grid_END/gridloss          5.10435e-03  1.94610e-02

Simple Rank Correlation Matrix among all inputs and outputs:
                          *rated_flow *hgap *beta_sp *k_void_drift *dhfrac */Grid_MID/gridloss *SpacerGrids/Grid_END/gridloss TotalPressure   MaxPinTemp
*CORE/rated_flow            1.00000e+00
*COBRATF/hgap               6.37347e-04  1.00000e+00
*COBRATF/beta_sp           -5.12786e-03 -1.72636e-02  1.00000e+00
*COBRATF/k_void_drift      -1.83830e-02  1.11400e-02 -1.16134e-02  1.00000e+00
*COBRATF/dhfrac             7.75866e-03 -4.44971e-03 -3.95800e-03 -1.43050e-03  1.00000e+00
*SpacerGrids/Grid_MID/gridloss          1.27543e-02  2.02847e-02  2.26627e-02  3.09793e-04  1.29317e-02  1.00000e+00
*/SpacerGrids/Grid_END/gridloss        -1.86462e-03  1.22835e-02 -9.04698e-03  2.07212e-02 -1.28511e-02 -2.14401e-02  1.00000e+00
TotalPressure               9.58944e-01  9.40477e-03  9.25357e-03 -1.38995e-02  1.28611e-02  2.85656e-01 -5.56802e-03  1.00000e+00
MaxPinTemp                 -1.72304e-01 -9.77567e-01  2.37077e-02 -9.80126e-03 -5.90689e-02 -2.22902e-02 -1.36460e-02 -1.73725e-01  1.00000e+00

Partial Rank Correlation Matrix between input and output:
                          TotalPressure   MaxPinTemp
*CORE/rated_flow            9.96970e-01 -8.52771e-01
*COBRATF/hgap               4.46931e-02 -9.94294e-01
*COBRATF/beta_sp            1.07805e-01  5.38069e-02
*COBRATF/k_void_drift       4.82002e-02 -1.93197e-02
*COBRATF/dhfrac             2.67128e-02 -5.09643e-01
*SpacerGrids/Grid_MID/gridloss          9.64687e-01  3.26336e-03
*SpacerGrids/Grid_END/gridloss          2.75427e-02 -2.52991e-02

                                                                                                                                                12175,0-1      99%
```

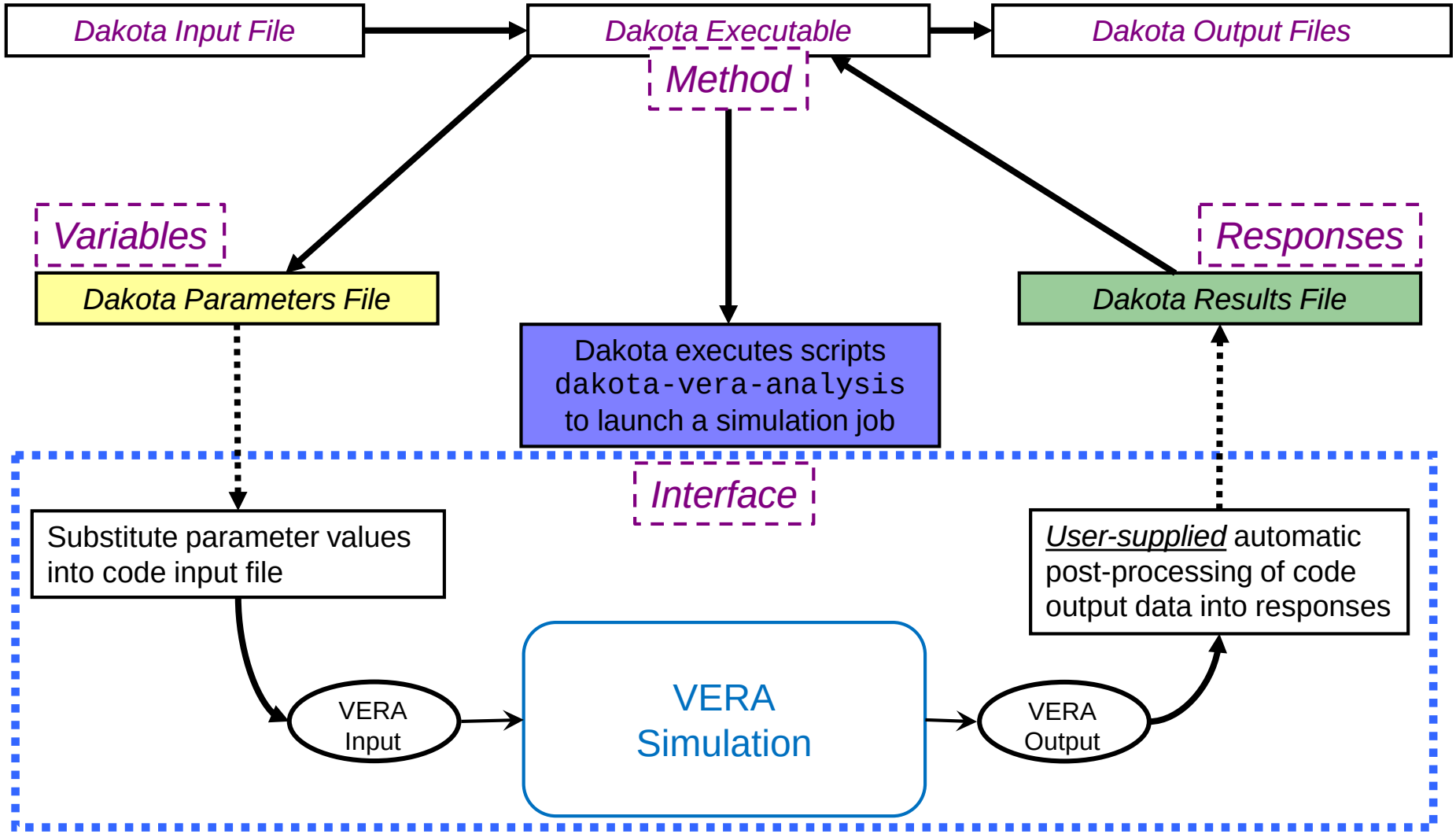
Exercise: Reliability

- Using a local reliability method in Dakota, estimate the probably of staying under or exceeding a (mock-) NRC operational limit:
  - Total Pressure Drop < 2.47 atm
  - Max Pin Temperature < 935 degC
- Modify the earlier UQ exercise to use a local reliability method
- Consider two cases for your input parameters:
  - a uniform distribution for your active parameters
  - a normal distribution for same
- Compare the results.
- Bonus: use the same samples from the earlier LHS study to build a PCE and get the statistics.

Module Learning Goal

- Understand the mechanics of how Dakota communicates with VERA simulations
  - May be beneficial in your project work
  - More extensive information in the Dakota Software Training: Interfacing to a Simulation slides on the Dakota website
  - Referenced Dakota to VERA adapter scripts are included in class materials as vuq_core

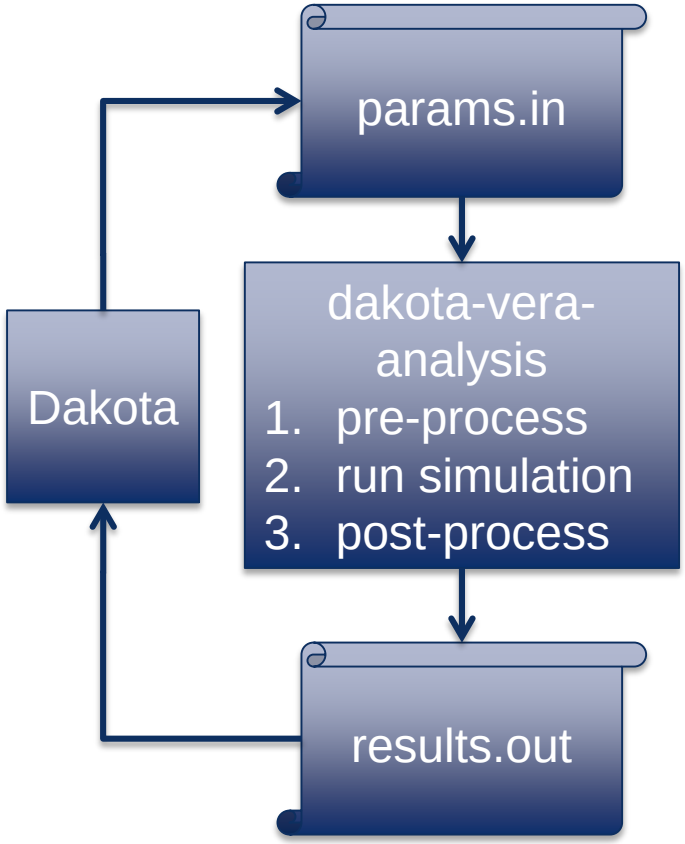
Dakota to Simulation Workflow



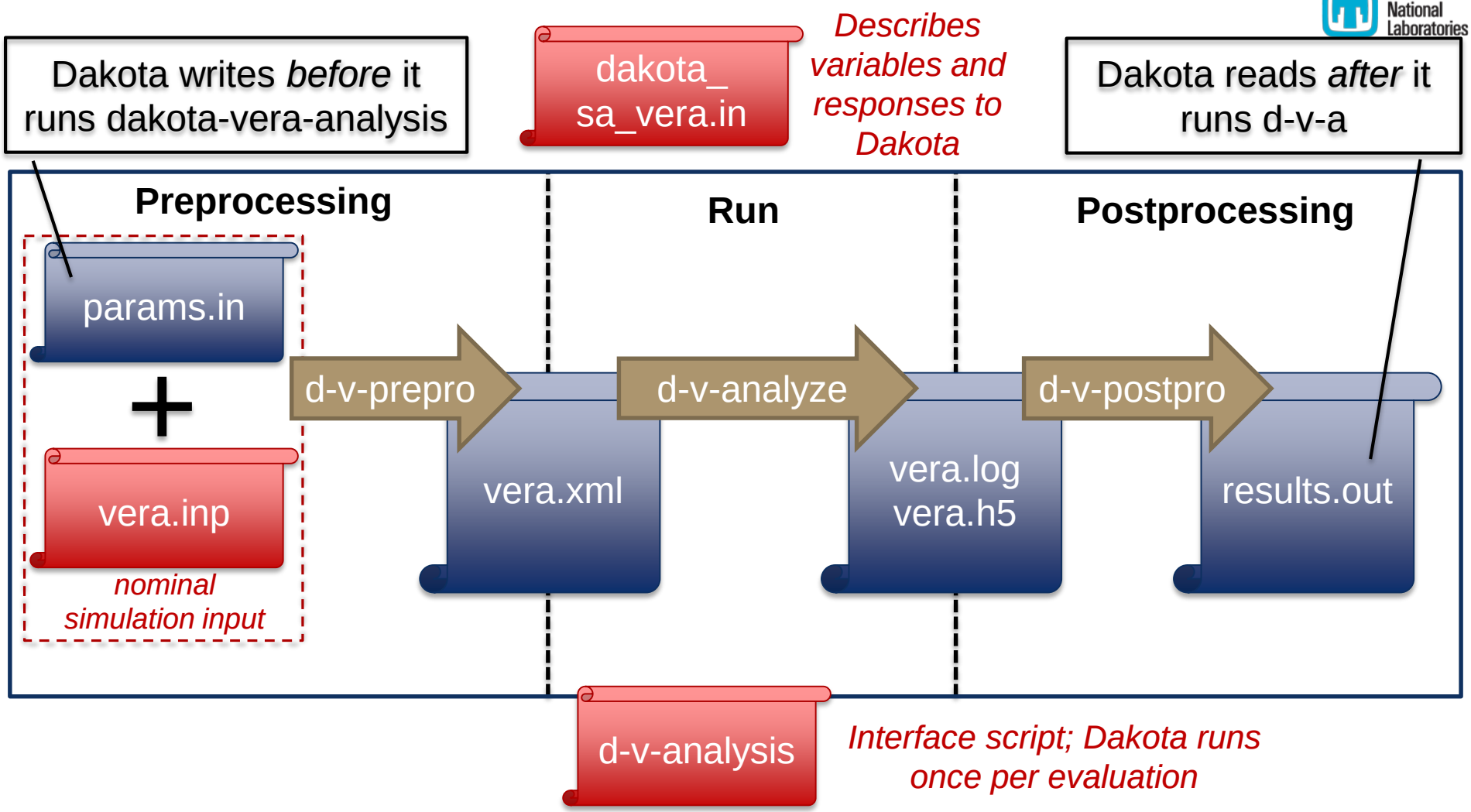
A Typical Dakota Evaluation in VERA

Each time Dakota wants to run a VERA simulation:

1. Dakota writes a parameters file that contains one value for each variable
2. Dakota invokes **dakota-vera-analysis**, passing it the names of the parameters and results files as command-line arguments
3. The dakota-vera-analysis driver performs three tasks to map parameters to results:
   1. **Pre-processing (dakota-vera-preprocess):** Create simulation input using values from the Dakota parameters file
   2. **Run (dakota-vera-analyze):** Run the simulation based on the input
   3. **Post-processing (dakota-vera-postprocess):** Extract scalar quantities of interest (responses) from simulation output and write them to the named Dakota results file
4. The user's interface exits
5. Dakota opens and reads the results file



VERA Interface Summary



Red….Created once, invariant
Blue…Changes every evaluation
Gold...Operations

Customizing the Workflow

- You can add your own post-processing scripts by naming them output_adapter* and placing alongside the Dakota input file
- More complex workflows such as including cross section library pertubations, model forms, or closure laws, require more advanced VUQ workflows not included in the examples.