Sandia National Laboratories

Dakota: Algorithms for Design Exploration and Simulation Credibility

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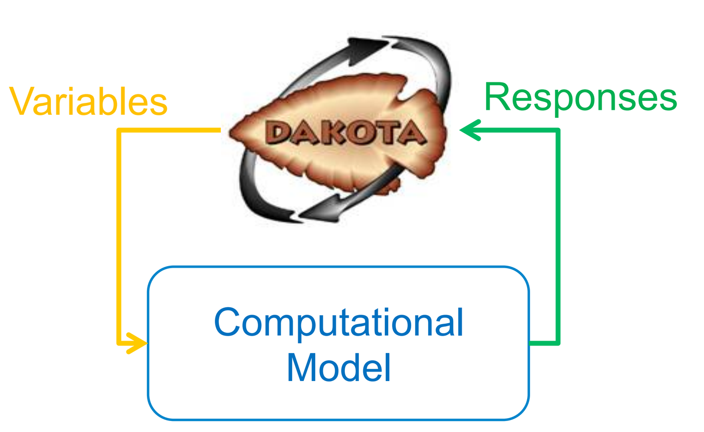
The **Dakota** toolkit provides a flexible, extensible interface between analysis codes and iterative systems analysis methods. Dakota contains algorithms for:

- Optimization with gradient and nongradient-based methods;
- Uncertainty quantification with sampling, reliability, stochastic expansion, and epistemic methods;
- Parameter estimation with deterministic (nonlinear least squares) and nondeterministic (Bayesian) methods; and
- Sensitivity/variance analysis with design of experiments and parameter study methods.

Methods may be used individually or combined into advanced workflows.

✓ Free & Open-source (LGPL)
✓ Scales from laptops to HPCs
✓ Portable (Windows, OS X, *NIX)

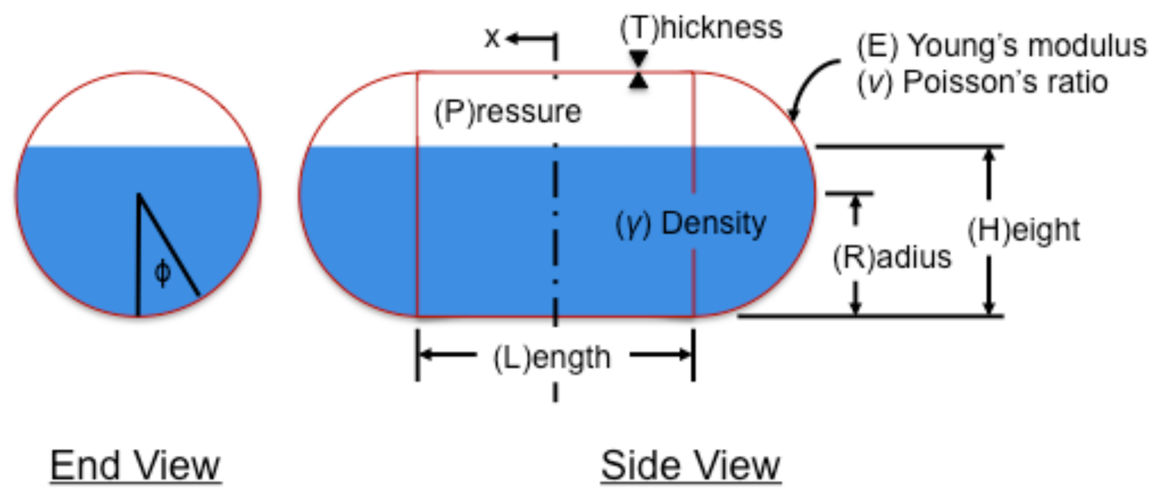


The Dakota toolkit recently was used to solve the 2014 Sandia National Laboratories Verification and Validation Challenge Problem.

Problem Statement

MysteryLiquid Co. maintains a large number of liquid-storage tanks. Standard operating procedures limit the maximum liquid level to a certain fraction of tank height. The headspace is filled with pressurized, inert gas.

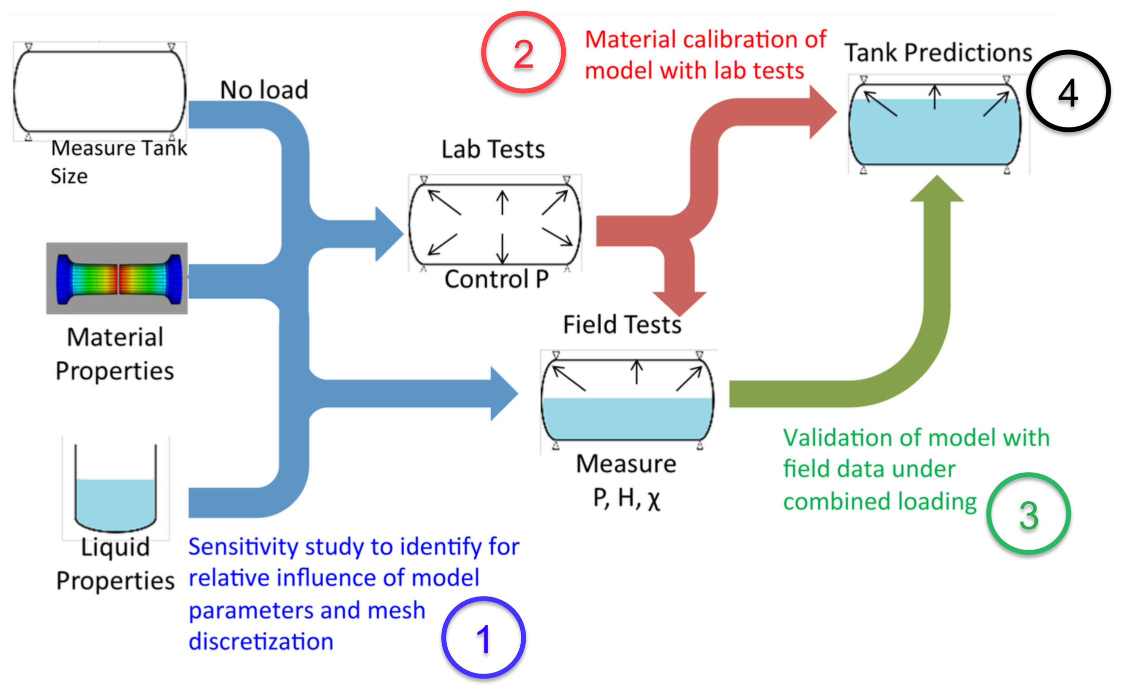
Recently, one of these tanks failed a routine safety inspection and consequently was taken out of service. *MysteryLiquid Co.* has commissioned experimental and modeling studies to determine whether the remaining tanks are safe to operate.



Specifically, what is the probability that the maximum von Mises stress exceeds the yield stress under nominal operating conditions?

Chain of Evidence

The figure to the right illustrates the sources and overall flow of information in the study. This information includes coupon tests, full-scale, pressure-only tank tests in the lab, and field observations of tank performance under combined liquid and pressure load.

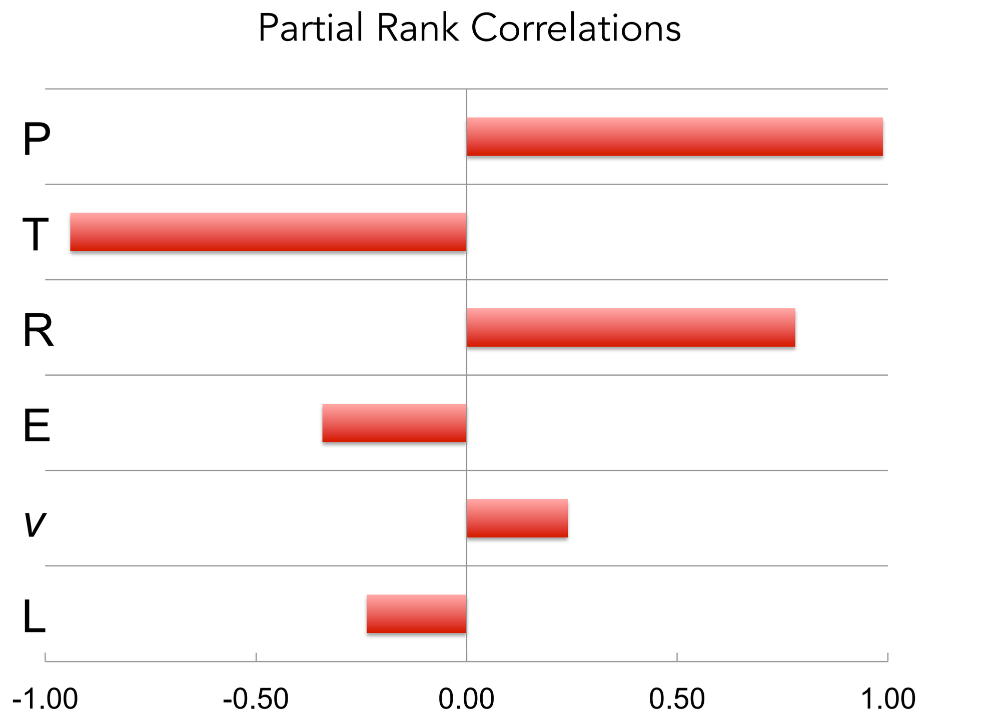


Sensitivity

Dakota's `sampling` method first was used to assess the sensitivity of the maximum von Mises stress to several parameters. Dakota computes a number of sensitivity metrics based on random sampling, including simple (Pearson's) and rank (Spearman's) correlations between all inputs and model responses. For both simple and rank correlations, Dakota also provides partial correlations.

Partial rank (Spearman's) correlations for the von Mises stress were computed from 16 Latin hypercube samples. Maximum stress occurred along the bottom of the tank (ϕ = 0) for all parameter sets. Correlations for maximum displacement were similar.

Although some parameters only weakly influenced the responses, all were included in the calibration.



Calibration

Dakota's least squares solver NL2SOL was used to identify model parameters. Because NL2SOL is a local optimizer, Dakota's `multi_start` feature was used to concurrently run ten separate calibrations from random initial points.

Dakota multi_start Specification

```
method
  id_method = 'ms'
  multi_start
    method_pointer = 'calib'
    random_starts = 10
```

Calibrated Parameters

Start	E (10^7)	v	L	R	T
1	3.00	0.28	59.51	29.70	0.23
2	2.89	0.29	59.54	29.44	0.23
3	2.77	0.29	59.66	29.44	0.24
4	2.69	0.29	59.66	29.44	0.25
5	2.84	0.29	59.59	29.44	0.23
6	2.62	0.29	59.59	29.44	0.25
7	2.57	0.29	59.82	29.44	0.26
8	2.98	0.29	59.52	30.37	0.23
9	2.73	0.29	59.67	29.44	0.24
10	3.07	0.28	59.47	29.44	0.22

Validation

Dakota's polynomial chaos expansion (PCE) capability was used to assess the validity of the tank model.

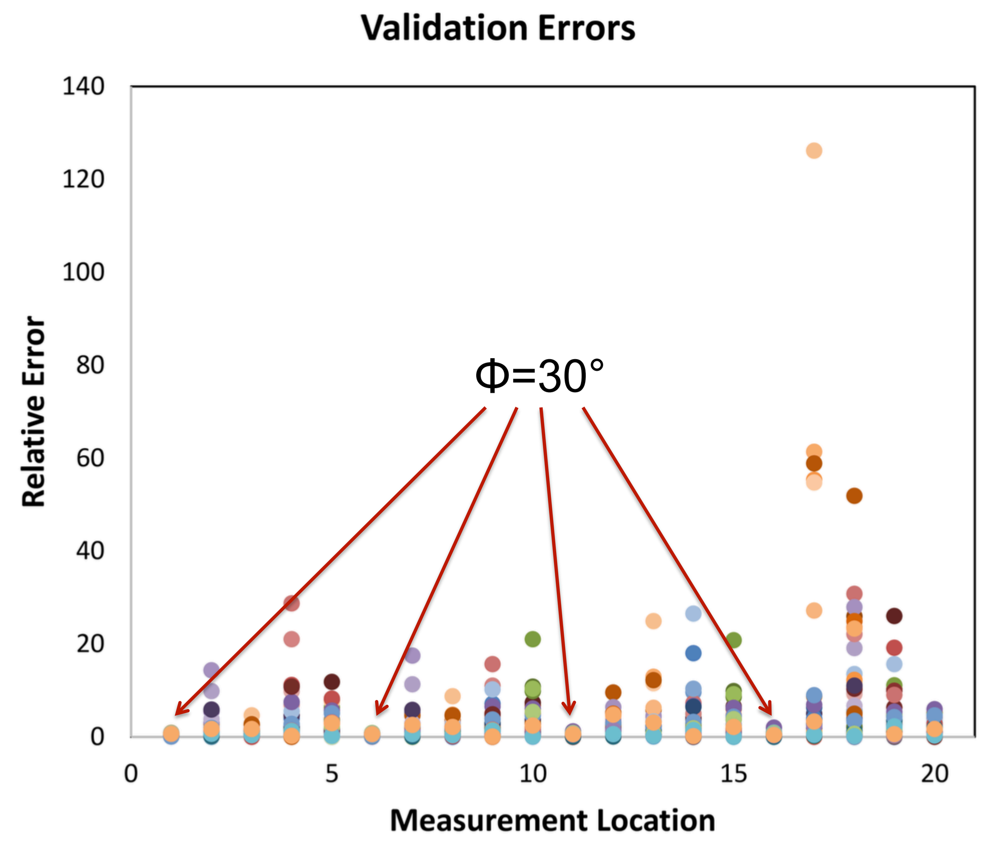
$$R = \sum_{j=0}^{P} \alpha_j \Psi_j(\xi)$$

A PCE is an approximate response constructed using global multivariate orthogonal polynomial basis functions defined over standard random variables.

A key feature of Dakota's PCE method is analytic variance-based decomposition, which produces Sobol indices. P, E, and T were revealed to contribute 63%, 16%, and 15%, respectively, to the variance of maximum displacement.

The PCE was sampled extensively over these three parameters at every tank surface location (ϕ, x) for which field observations were available, and a relative error between the PCE prediction and observation was computed for each sample. The errors are plotted in the figure below.

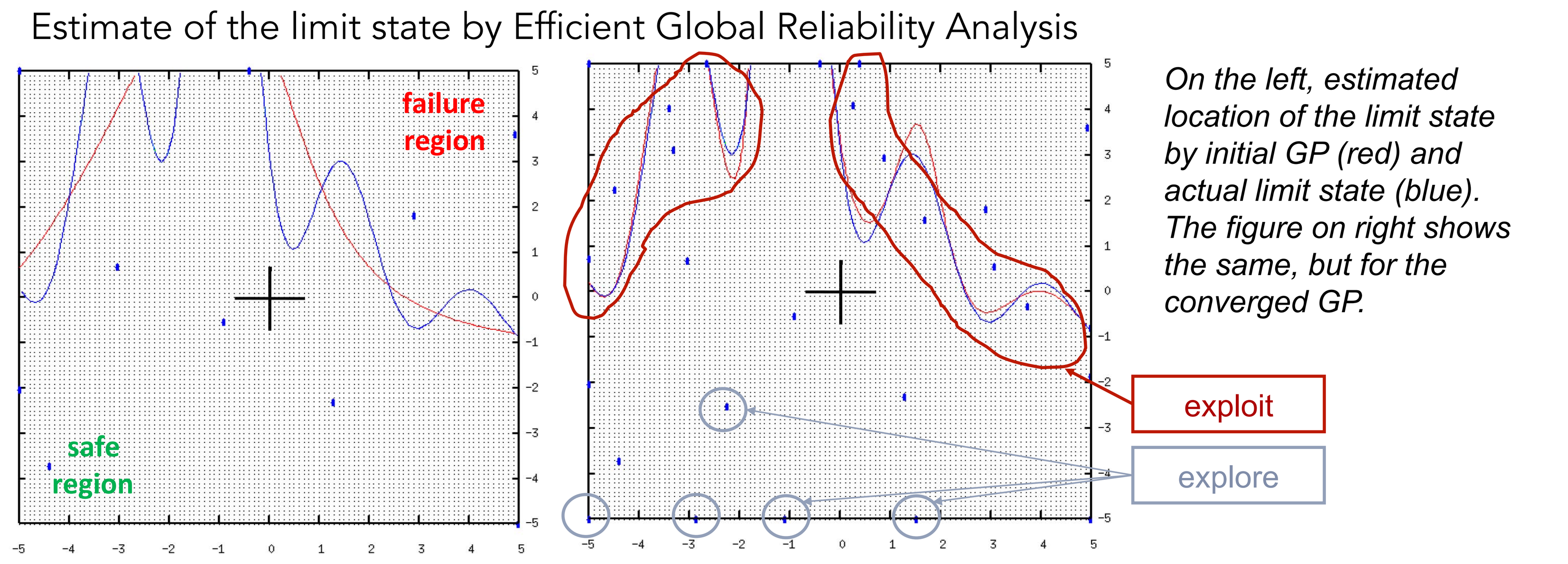
Validation errors were lowest at locations 1, 6, 11 and 16. Of the field data provided, these locations were the nearest to ϕ = 0°, where the model predicts the greatest stress and displacement occurs. This raises confidence in failure probability estimates based on the model. However, large errors at other locations remain unexplained. These errors coupled with a lack of observation data along the bottom of the tank tend to undermine confidence in the adequacy of the model.



Reliability

Probability of failure was estimated using Dakota's Efficient Global Reliability Analysis (EGRA) algorithm. EGRA constructs and iteratively improves a Gaussian process (GP) approximation with the goal of increasing accuracy in the region of the limit state—in this case, the boundary in E-T space where the von Mises stress equals the yield stress. Importance sampling is then performed on the converged GP is used to estimate probability of failure.

Estimate of the limit state by Efficient Global Reliability Analysis



On the left, estimated location of the limit state by initial GP (red) and actual limit state (blue). The figure on right shows the same, but for the converged GP.

For the ranges of Young's modulus and tank thickness considered, it was found that there was no possibility (0 probability to within machine precision) of the maximum von Mises stress exceeding the yield stress.

Dakota played an integral role at all stages of addressing the V&V Challenge problem

- ❖ Dakota algorithms for sensitivity analysis, calibration, and reliability were brought to bear on different aspects of the problem, all with minimal changes to the Dakota input and Dakota-model interface.
- ❖ Auxiliary Dakota components such as surrogate models and parallel execution management significantly reduced the number of model runs and wall clock time to solution.

The Dakota team works continually to further streamline analysis workflows and guide users to the appropriate Dakota capabilities based on their goals, model characteristics, and computational resources and budgets. Recent efforts include:

- ❖ Roll-out of a Dakota web portal (https://dakota.sandia.gov) that will host forums, areas for user-submitted content, tutorials, and other community-oriented elements
- ❖ Updated activity-based training materials—videos of recent training sessions are now available on the Dakota web portal
- ❖ Ongoing development of a new GUI that will simplify and enhance Dakota by providing readily accessible examples, contextual access to documentation, follow-on analysis and plotting of Dakota results, and more

References

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