SAND2014-4259C

Surrogate-Based V&V

Lauren L. Beghini, Patricia D. Hough

Sandia National Laboratories

Sandia National Laboratories

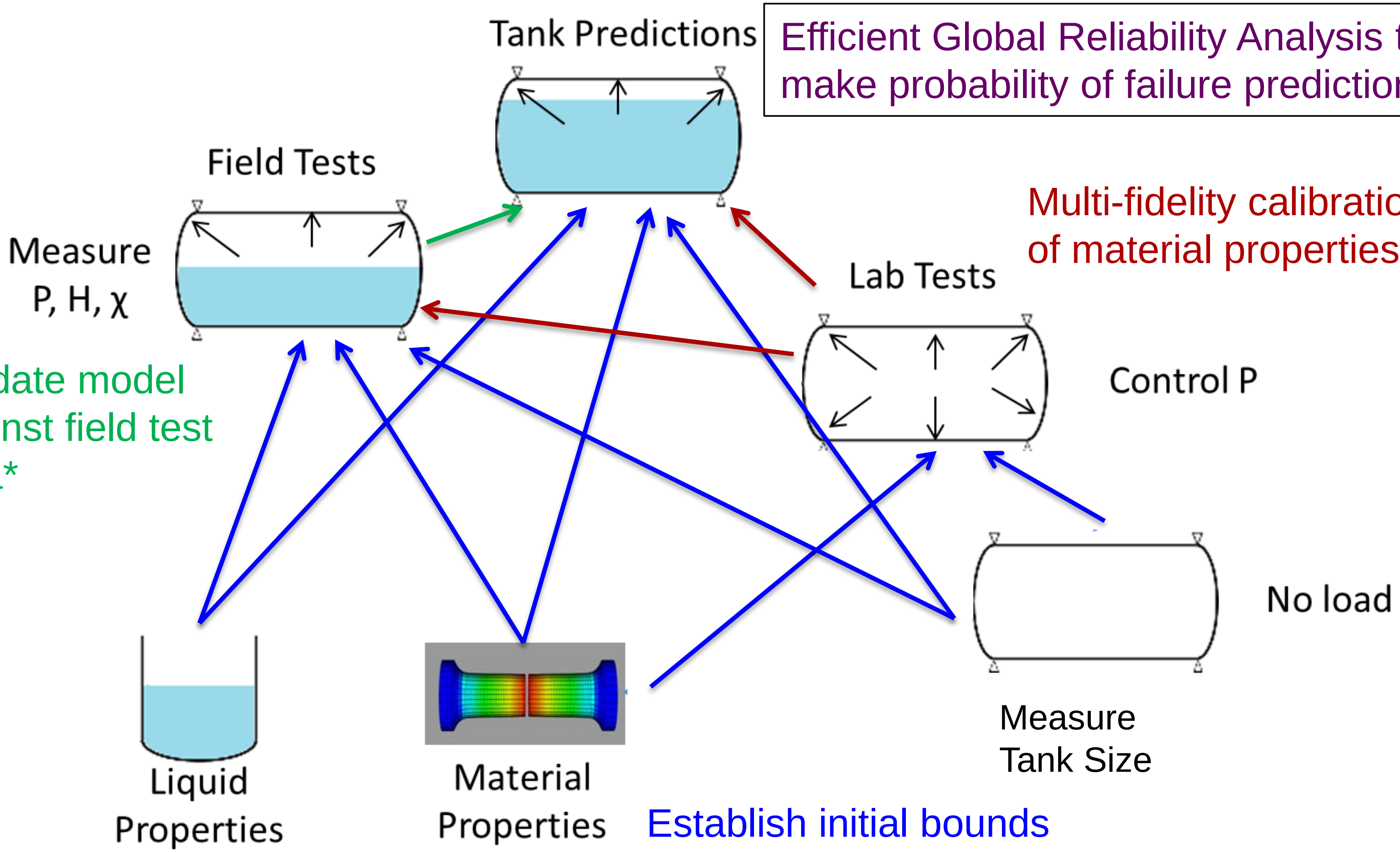
Exceptional service in the national interest

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

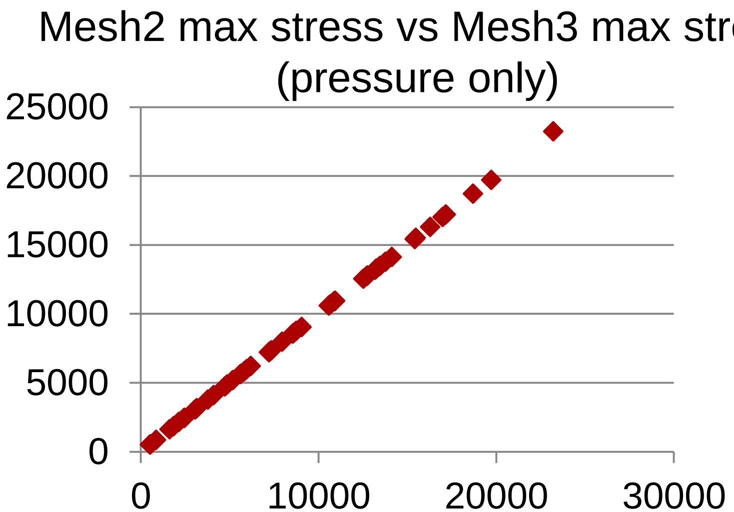
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2013-1715P

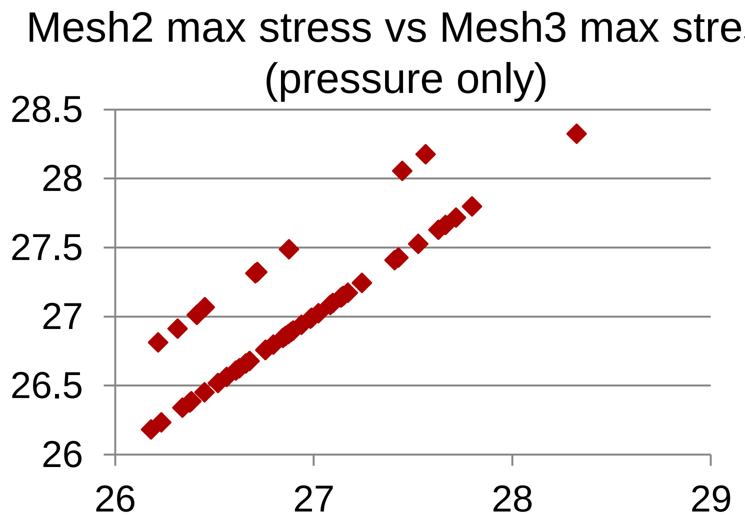
Goal is to use response surface and multi-fidelity surrogates to minimize number of simulations



*Used polynomial chaos expansions for higher-order sensitivity analysis

Small initial LHS study established relationship between model fidelities

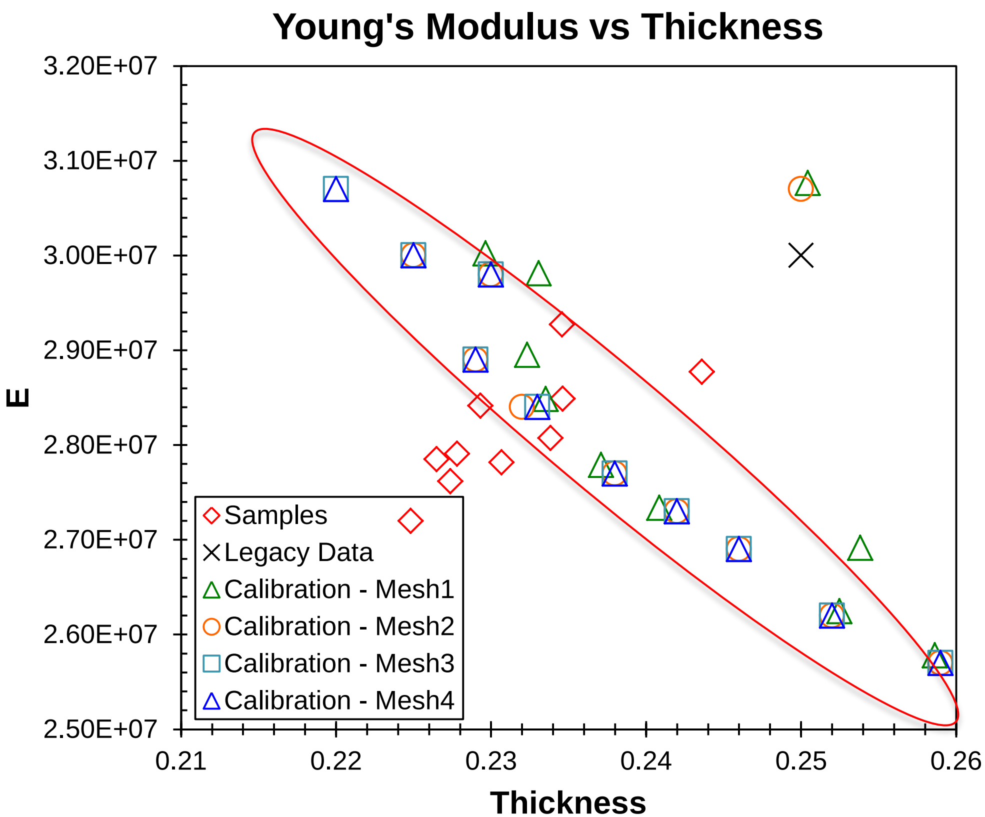




- Max stress and displacement values were consistent across fidelities
- Location of max stress varied but in a reasonably nice way
  - Most difference between Mesh2 and Mesh3
- Observations support multi-fidelity calibration approach
- Number of simulations
  - Mesh4 = 6
  - Mesh3 = 48
  - Mesh2 = 384
  - Mesh1 = 384

Calibration progressed from Mesh1 to Mesh4 – and don’t forget about scale…

Sandia National Laboratories



- Used multi-start least-squares solver
  - Calibrated Mesh1 (71 runs)
  - Fed solutions forward to calibrate Mesh2 (49 runs)
  - Then to Mesh3 (45 runs)
  - And finally Mesh4 (42 runs)
- Noticed inconsistency with material data
- Scaling parameters reduced inconsistency but converged to only one solution

Polynomial chaos expansion was used to compute higher-order sensitivities

Approximate response with Galerkin projection using global multivariate orthogonal polynomial basis functions defined over standard random variables

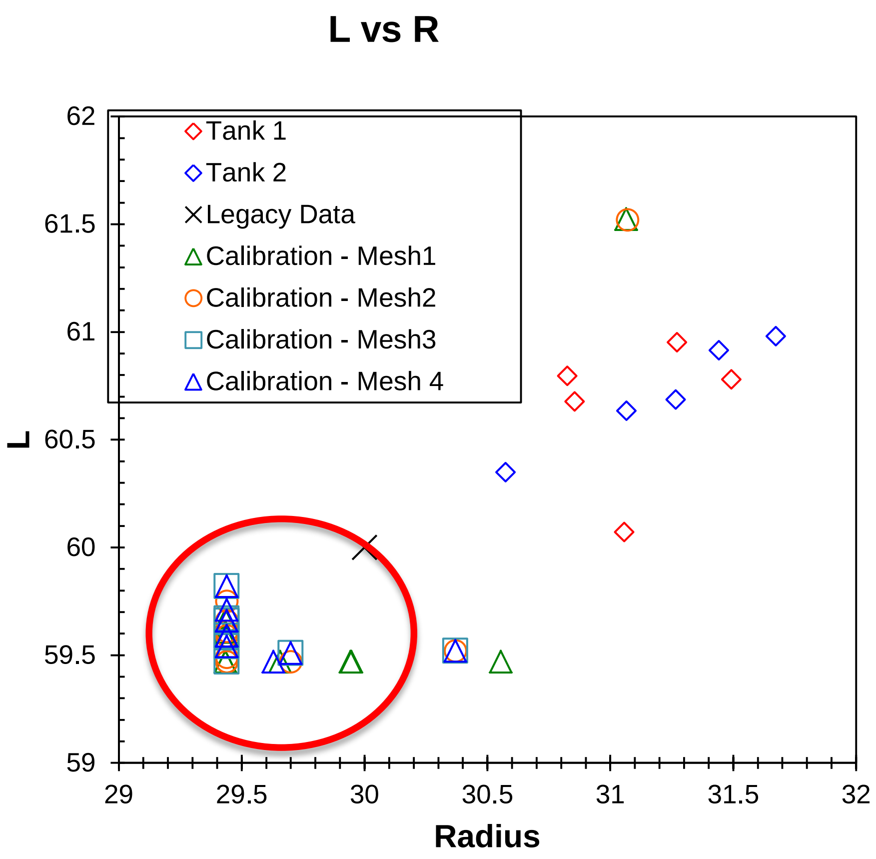
$$R = \sum_{j=0}^{P} \alpha_j \Psi_j(\xi)$$

R(ξ) ≈ f(u)

$$\alpha_j = \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} = \frac{1}{\langle \Psi_j^2 \rangle} \int_{\Omega} R \, \Psi_j \, \varrho(\xi) \, d\xi$$

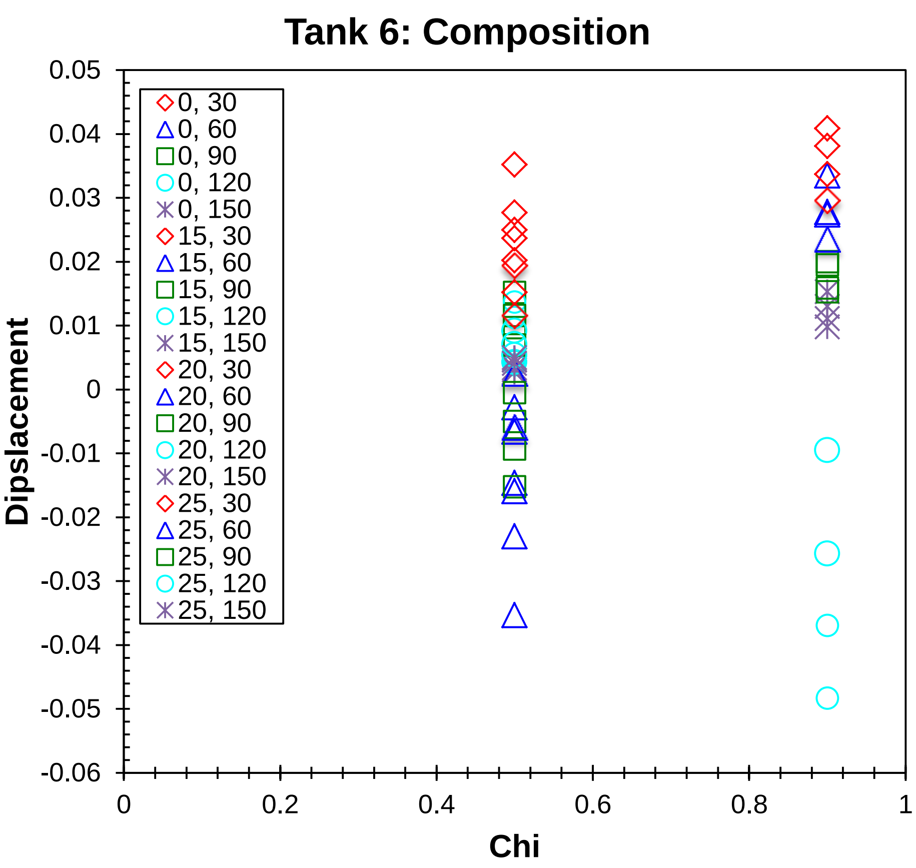
- One approximated, calculate statistics (and sensitivities) analytical, or sample the cheaper surrogate.
- Wiener-Askey Generalized PCE: optimal polynomial basis leads to exponential convergence of statistics (Normal/Hermite, Uniform/Legendre)

Higher-order sensitivities helpful in ruling out interactions of tank dimension with materials



- Noticed that calibration consistently identified smallest tank length and radius
- Sensitivities ruled out second- or third-order interactions
  - Based on polynomial chaos expansion
  - Re-used LHS samples, so no additional simulations
- Possible improvements
  - Calibrate material properties over uncertain tank dimensions
  - Split data and use part for intermediate validation

Validation activities were limited



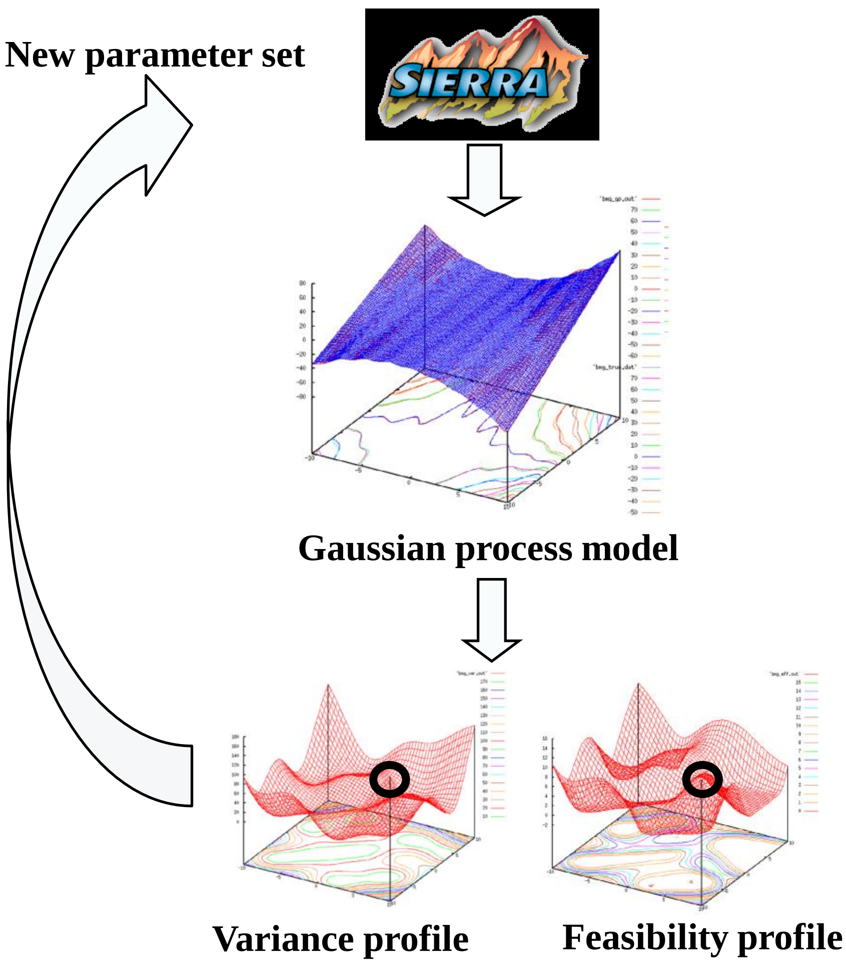
- Data requires careful study
  - Coverage of domain
  - Confounding of effects
- Ran sensitivity study similar to that for pressure-only case
- Metric would likely emphasize bottom of tank but include all locations
- Possible improvement
  - Split data and also calibrate liquid properties
- Ran into one big issue…

Code Verification Anyone?
When upper bound on H > 50 …

```
Traceback (most recent call last):
  File "/home/pdhough/Projects/VVTankProblem/DakotaLHSLiquid_breakit//EvalTank.py", line 150, in <module>
    main()
  File "/home/pdhough/Projects/VVTankProblem/DakotaLHSLiquid_breakit//EvalTank.py", line 144, in main
    FEMTank.main(X_vec, Phi_vec, Pressure, Gamma_Chi, LiqHeight, E, Nu, Length, Radius, Thickness, meshID, summaryFileName, dataFileName)
  File "/home/pdhough/Projects/VVTankProblem/DakotaLHSLiquid_breakit/FEMTank.py", line 830, in main
    results = cylinder(X_vec_new, Phi_vec_new, Pressure_new, Gamma_new, LiqHeight_new, E_new, Nu_new, Length_new, Radius_new, Thickness_new, M, N, '','') # don't have cylinder write any files
  File "/home/pdhough/Projects/VVTankProblem/DakotaLHSLiquid_breakit/FEMTank.py", line 616, in cylinder
    results = cylEvalResults(M, N, X_vec, Phi_vec, Length, Thickness, Radius, E, Nu, Pressure, Gamma, LiqHeight)
  File "/home/pdhough/Projects/VVTankProblem/DakotaLHSLiquid_breakit/FEMTank.py", line 497, in cylEvalResults
    D_fluid_mn = cylEvalLoadCoeff_fluid_mn(Radius, gamma, LiqHeight, m, n)
  File "/home/pdhough/Projects/VVTankProblem/DakotaLHSLiquid_breakit/FEMTank.py", line 440, in cylEvalLoadCoeff_fluid_mn
    alpha = pi-acos((LiqHeight-Radius)/Radius)
ValueError: math domain error
```

Used Efficient Global Reliability Analysis (EGRA) for probability of failure estimates

Sandia National Laboratories



- Iteratively refines Gaussian process
- Balances exploration of unknown space with refinement around threshhold
- Spent too many simulations exploring

Bichon, B.J., Eldred, M.S., Swiler, L.P., Mahadevan, S., and McFarland, J.M., "Efficient Global Reliability Analysis for Nonlinear Implicit Performance Functions," *AIAA Journal*, Vol. 46, No. 10, October 2008, pp. 2459-2468.

Gaussian process is a stochastic process defined by mean and covariance functions

Sandia National Laboratories

- Can have constant, linear, and quadratic mean trend

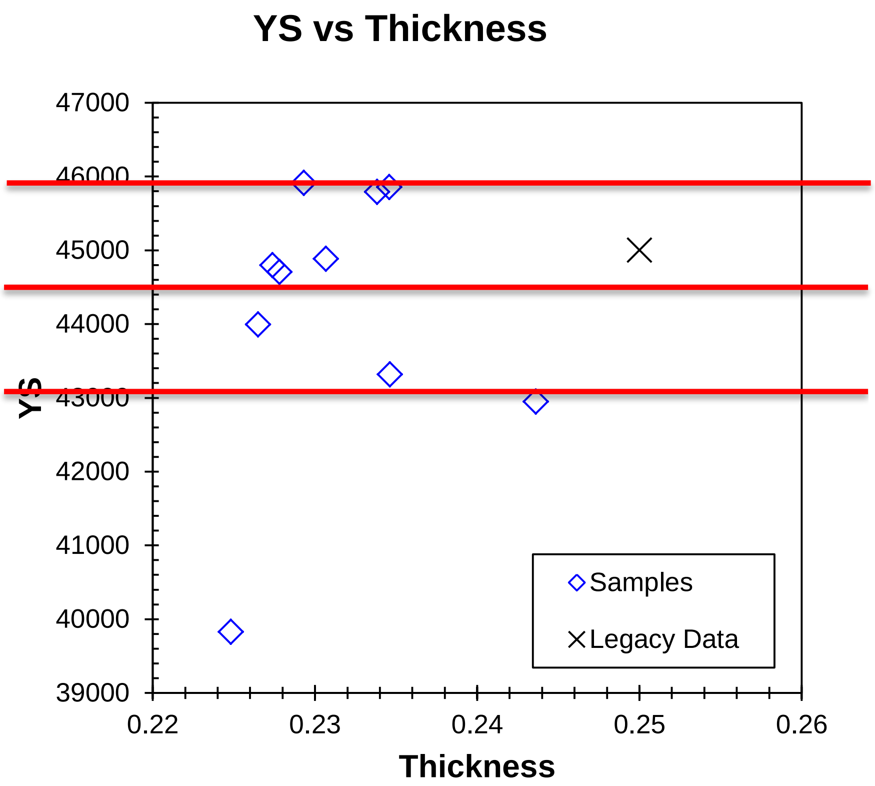
- Covariance function is

$$C_{12}(\mathbf{x}^1, \mathbf{x}^2) = \sigma^2 \exp\{-\sum_{i=1}^{n} \rho_i^2 (\mathbf{x}_i^1 - \mathbf{x}_i^2)^2\}$$

where σ and ρ_i are found by maximizing the likelihood function

$$L = \frac{-n}{2}\log(2\pi) - \frac{1}{2}\log(\det(C)) - \frac{1}{2}\mathbf{z}^T C^{-1}\mathbf{z}$$

Probability of failure at nominal test conditions came out to be 0!?!?!



- Considered three different failure threshholds
- Also considered threshhold of 20,000
  - Exceeded with probability 1
- 50 (unique) simulations using Mesh3

Do we consider the model credible enough to base a decision on?

Sandia National Laboratories

- Geometric fidelity – not enabled by this activity
- Physics fidelity – low, by definition
- Solution verification – relationship between meshes understood
- Code verification – code crashes for some of parameter range
- Validation – insufficient time spent on it
- Uncertainty quantification – some done, incomplete for validation, no roll-up (need to include surrogate errors)

- NO, especially given limited historical experience with model
- Want to prioritize and request resources to address most pressing model and data needs