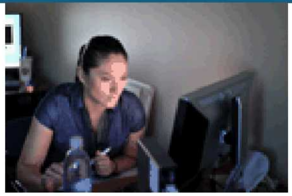
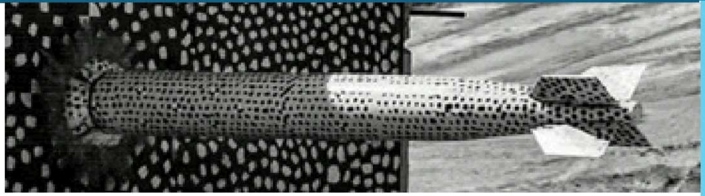
SAND2019-8550C

Survey of DAKOTA's V&V Capabilities in the Simulation of Residual Stresses in a Simple Composite Structure





Stacy Nelson and Alexander Hanson

Sandia National Laboratories, Livermore, CA

15th U.S. National Congress on Computational Mechanics
July 28-August 1, 2019, Austin, TX

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

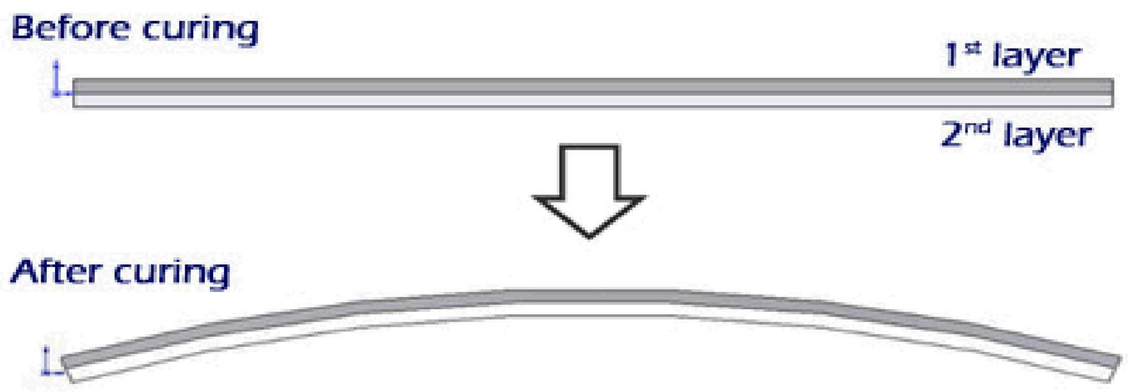
Presentation Outline

- Background
  - Why do we care about residual stresses?
  - How are residual stresses modeled?
  - Motivation and objectives for this study
- Methodology - What is an efficient validation procedure for process-induced stresses?
  - Validation Experiments
  - Finite Element Methods
  - Solution Verification and Mesh Optimization
  - Survey of DAKOTA's Validation Methods
- Conclusions
  - Summary of results
  - Ideal validation approach

Background

Why do we care about residual stresses?

- Hybrid composites are used in many structural applications
  - Lamination of fiber composites, metals, plastics, and paints
  - Exploit materials strengths, but exhibit pronounced process-induced stresses
- Residual stresses develop due to:
  - Differences in the curing conditions
  - Coeff. of thermal expansion mismatch
  - Polymer shrinkage



- Residual stresses manifest as:
  - Physical deformation and warpage
  - Interlaminar delamination
- Experimental quantification of residual stresses is expensive
  - Validated modeling methods are preferred and can be applied to any structure

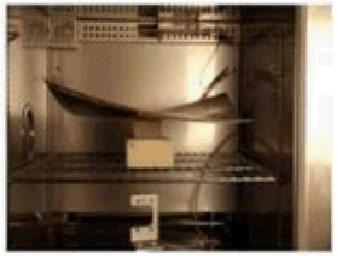
How do we quantify residual stresses?

- Experimental quantification of residual stresses is expensive
  - Validated modeling methods are preferred and can be applied to any structure
- Two common approaches to simulating residual stresses in composite structures:
  - Method 1: Complex → Complete curing process
    - At least 45 parameters, several for calibration
  - Method 2: Simple → Simplified curing process
    - Only 13 parameters, all can be experimentally determined
    - Sandia's selected approach for efficiency and suitability to structures of interest

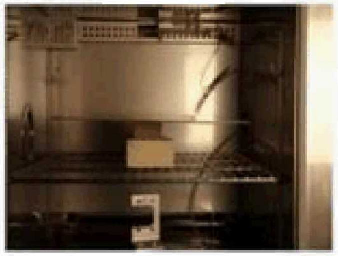
A Method to Predict Residual Stresses in Hybrid Composites

- Stress-free temperature experiment
  - Indicates when thermal strains should develop
  - Accounts for polymer shrinkage
- Approximated composite curing cycle in two consecutive simulations
  - Simulation Process:
    - Composite is uncured, compliant, isotropic
    - Isothermal heating from ambient to stress-free temperature
    - Composite material is "activated" with room temperature, orthotropic material properties
    - Isothermal cooling from stress-free temperature to ambient
    - Differential thermal strains develop and residual stresses are formed

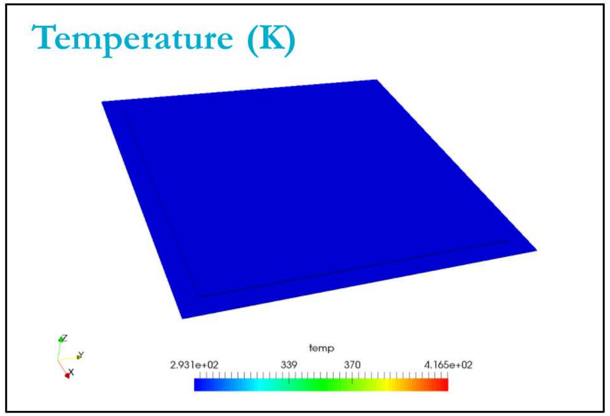
Experimental Determination of T_{SF}



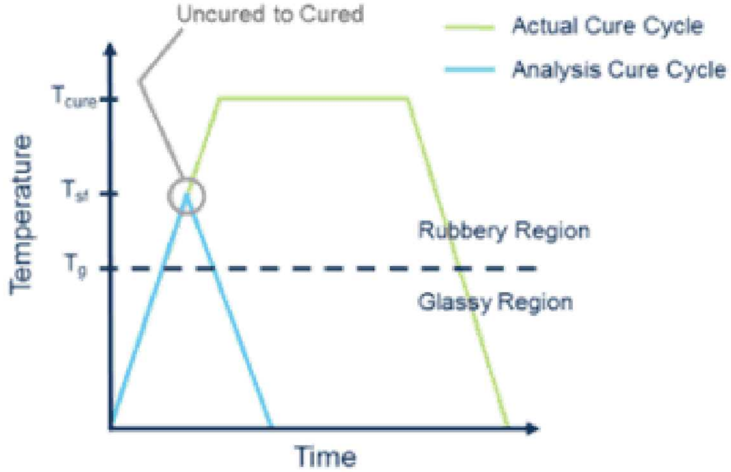
50°C



140°C



Real and Simulated Curing Cycles

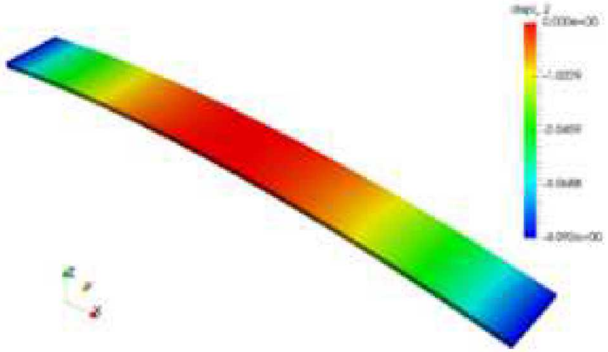


Validation of the Residual Stress Modeling Approach

- Four validation challenge problems
  - Relevant materials
  - Measurable residual stress driven deformation
  - Industry relevant geometries
- Modeling approach is well validated and robust
  - All predictions were mesh convergent and within 10% of measurement
  - Strip/bracket made from different material than plate/rings
  - Formal sensitivity studies and UQ were applied to plate and ring
    - What material parameters are most important?
    - How does parameter uncertainty affect predictions?

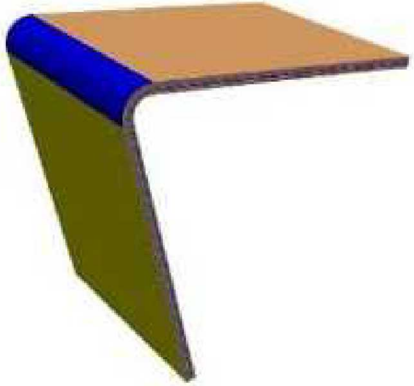
Asymmetric Composite Strip

Prediction within 2% of measured

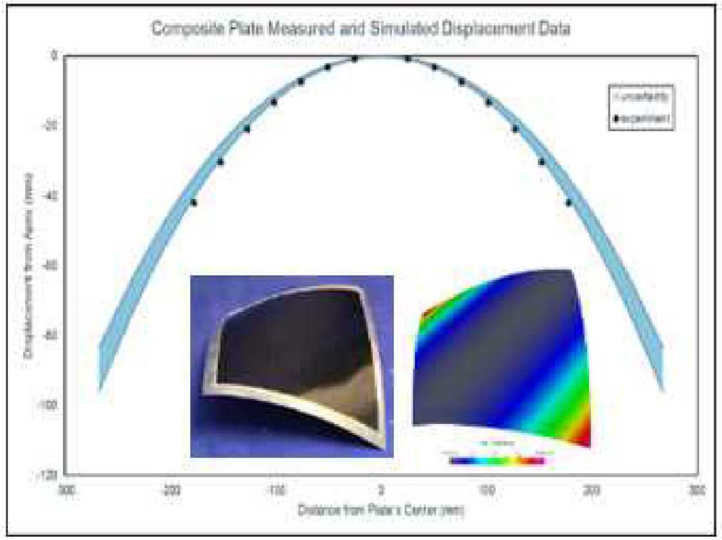


Composite Angle Bracket

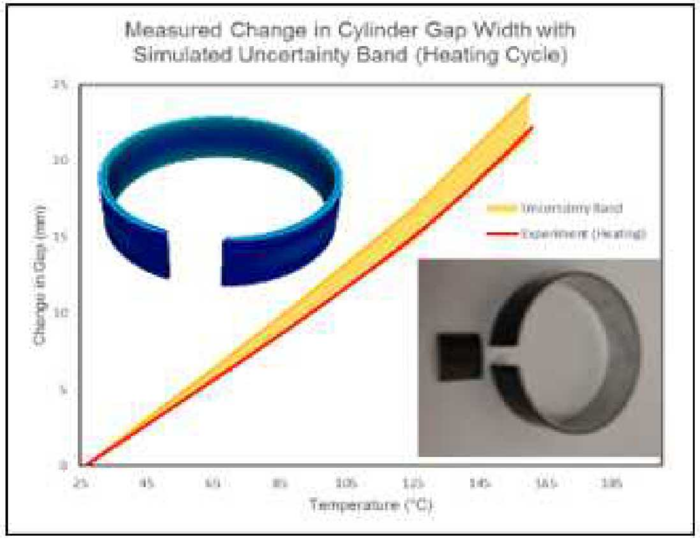
Prediction within 8% of measured



Bi-Material Plate



Bi-Material Split-Rings



*Nelson, S., Hanson, A., Briggs, T., Werner, B., "Verification and Validation of Residual Stresses in Composite Structures," Composite Structures, v194, p662-673.

Motivation and Objectives

- Motivation:
  - Modeling and simulation is increasingly being used to support the qualification of complex composite parts
  - Component level models are too expensive for traditional sampling methods
- Objectives:
  - Develop a residual stress case study that will be:
    - Low-cost to model → Sensitivity studies will require thousands of simulations
    - Reasonable to physically implement → nominal model validation is important
  - Complete a survey of common sensitivity analysis methods
    - What parameters are critical to the stress predictions?
  - Complete a survey of common UQ methods
  - What is the most efficient validation method for the hybrid composite structures?

Methodology

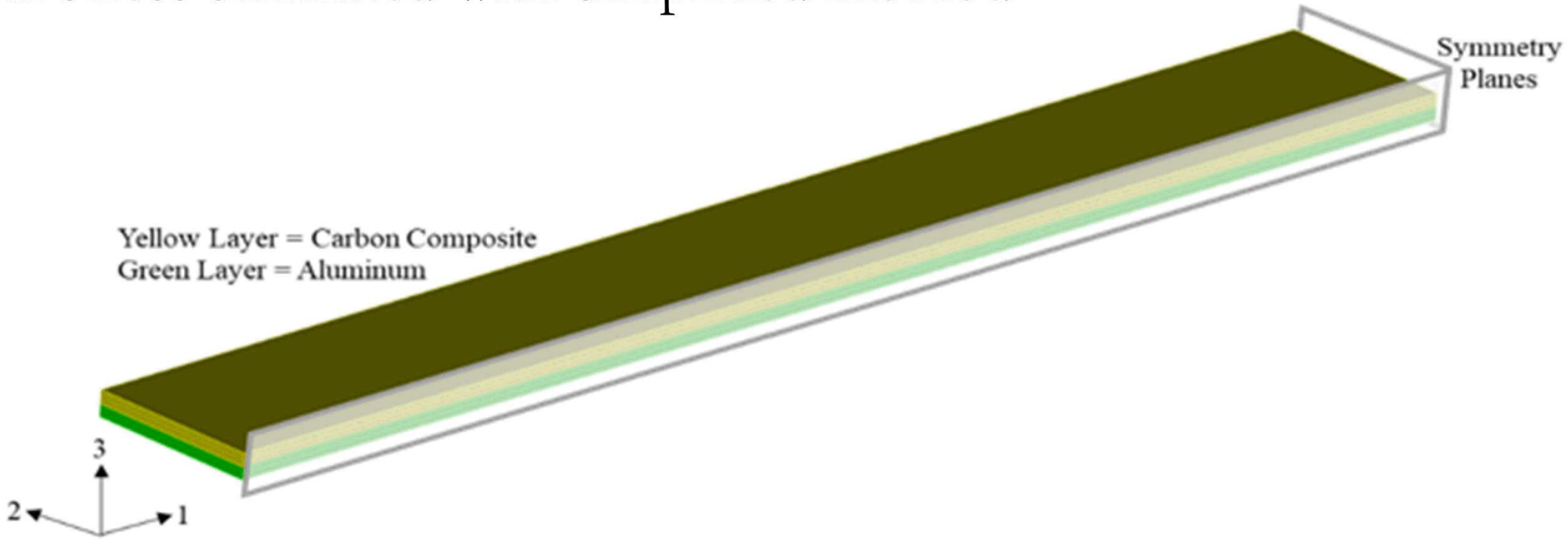
Validation Experiment

- Bi-material, composite/aluminum strip
  - Efficient and low-cost to model
  - Process-induced stresses manifest as out-of-plane warpage/curling along the strip's length
- Materials:
  - Carbon composite and Aluminum
  - Composite co-bonded to aluminum

- Measurement procedure:
  - Granite table, guarantees flatness
  - Digital height gage, ±0.01 mm
- Two types strips manufactured and measured
  - Shorter strip for sensitivity study → 11.01mm
    - Limited experimental rigor expended, sensitivity study is not validation
  - Longer strip for UQ → 26.41 ± 0.21 mm

Model Geometry and Boundary Conditions

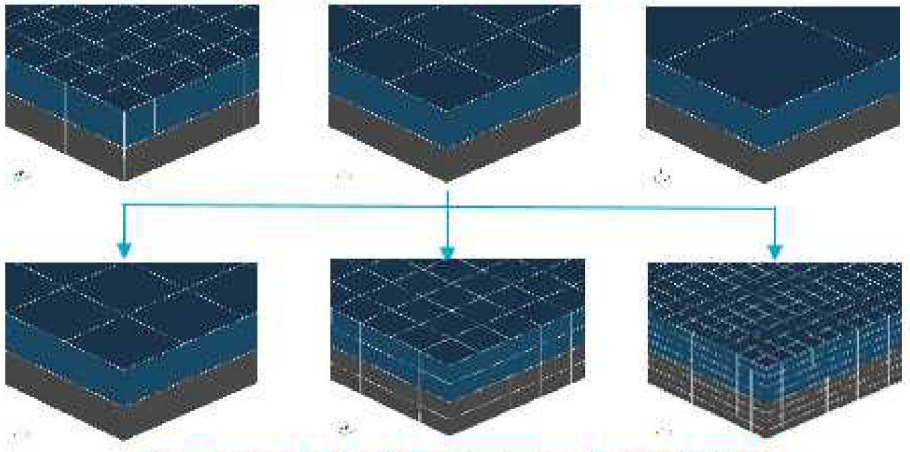
- Aluminum/carbon composite modeled as separate, homogenized material layers
- Carbon composite layer merged to aluminum layer
  - Merging approximates perfect bonding, delamination is not modeled
- Boundary conditions:
  - Quarter model symmetry conditions assumed for computational efficiency
  - Residual stress simulated with simplified method



Solution Verification, Mesh Optimization, Nominal Model Validation

- Mesh study considered element size and aspect ratio
  - What is the largest element providing confident predictions?
- 3 element lengths and 3 aspect ratios
  - 9 models processed according to described methods
  - 3 separate mesh studies based on the 3 aspect ratios
- Richardson's extrapolation estimated "exact" out-of-plane displacement
  - Approximates a higher order estimate of a continuum value given discrete solutions → discretization errors
- Summary of results:
  - Extrapolated exact solutions do not differ significantly
    - 1:4:4 can be used with a reasonable expectation of model accuracy
  - Medium, 1:2:2 mesh size offers best combination of computational efficiency and model accuracy
    - Lowest discretization error with fewer than 36 solution cores
    - Exact solution and shape of deformation agree well enough with experiment to satisfy physics

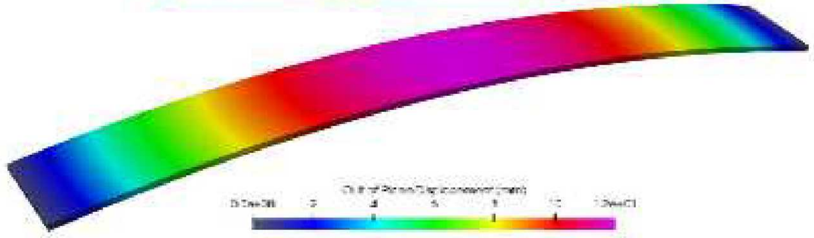
3 Element Aspect Ratios and 3 Levels of Refinement



Summary of Mesh Convergence Study Results

Aspect Ratio	Mesh Refinement Level	Run Time (min) /Solution Cores	Predicted Deflection (mm)	Error (%)	Exact Solution (mm)
1:1:1	Coarse	01:14.3/1	14.02	20.2	11.666
	Medium	04:51.7/4	12.16	4.3	
	Fine	24:32.7/36	11.77	0.9	
1:2:2	Coarse	00:33.7/1	12.75	9.4	11.652
	Medium	**01:04.4/4**	**11.90**	**2.2**	
	Fine	03:24.3/36	11.71	0.5	
1:4:4	Coarse	00:25.2/1	9.33	20.3	11.702
	Medium	00:40.1/4	10.94	6.5	
	Fine	00:59.7/36	11.46	2.1	

Representative Deformation Prediction



Overview of Completed Surveys

- What is the most computational efficient validation procedure?
  - Sensitivity study and UQ
- Six sensitivity study methods were examined:
  - Parameter study (centered parameter study(CPS))
  - Design of Experiments (Box-Behnken Design (BBD))
  - Sampling Methods (Monte Carlo (MC), Latin HyperCube (LHS))
  - Surrogate Methods (Gaussian process (GP), Polynomial Chaos Expansion (PCE))
- Four UQ methods were examined:
  - Sampling Methods (Monte Carlo, Latin HyperCube)
  - Surrogate Methods (Gaussian process, Polynomial Chaos Expansion)
- Approach to completing the survey:
  - Step 1: Define parameter space
    - Nominal values ± 3 standard deviations *or* ± percentage of the nominal
  - Step 2: Complete sensitivity studies with the six methods
  - Step 3: Complete N-way ANOVA to find critical parameter list
  - Step 4: Complete UQ with the four methods
  - Step 5: Calculate means, standard deviations from distribution of predictions

Sensitivity Study Parameter Space

	Parameter	Minimum Value	Maximum Value
Composite Properties	E_{11} (GPa)	57.5	70.2
	E_{22} (GPa)	56.5	69.0
	E_{33} (GPa)	7.7	9.4
	ν_{12}	0.043	0.053
	ν_{13}	0.367	0.449
	ν_{23}	0.367	0.448
	G_{12} (GPa)	3.1	3.8
	G_{13} (GPa)	2.9	3.6
	G_{23} (GPa)	2.9	3.6
	T_g (°C)	110.9	141.8
	T_{sf} (°C)	140.6	146.1
	CTE_{11} (1/°C, rubbery)	0.294e-6	1.913e-6
	CTE_{22} (1/°C, rubbery)	0.357e-6	2.794e-6
	CTE_{33} (1/°C, rubbery)	268.1e-6	290.9e-6
	CTE_{11} (1/°C, glassy)	3.060e-6	3.708e-6
	CTE_{22} (1/°C, glassy)	2.585e-6	4.165e-6
	CTE_{33} (1/°C, glassy)	67.8e-6	76.5e-6
Aluminum Properties	E (GPa)	57.0	85.6
	ν	0.264	0.396
	CTE (1/°C)	18.7e-6	28.1e-6

Results

Comparison of Sensitivity Analysis Methods

- Surrogate methods require the fewest samples for a converged list of critical parameters
- Sampling methods are the least efficient approaches → 4-8x more expensive than surrogate methods
  - Simple to implement without access to DAKOTA
- BBD is more efficient than the sampling methods, but twice as expensive as the surrogate methods
  - Can be implemented without access to DAKOTA
- CPS provides a reasonable critical parameters list at a low number of samples, but seems to omit some of the less influential critical parameters
  - Should be considered when a measure of sensitivity is required, but only a handful of samples are computationally affordable

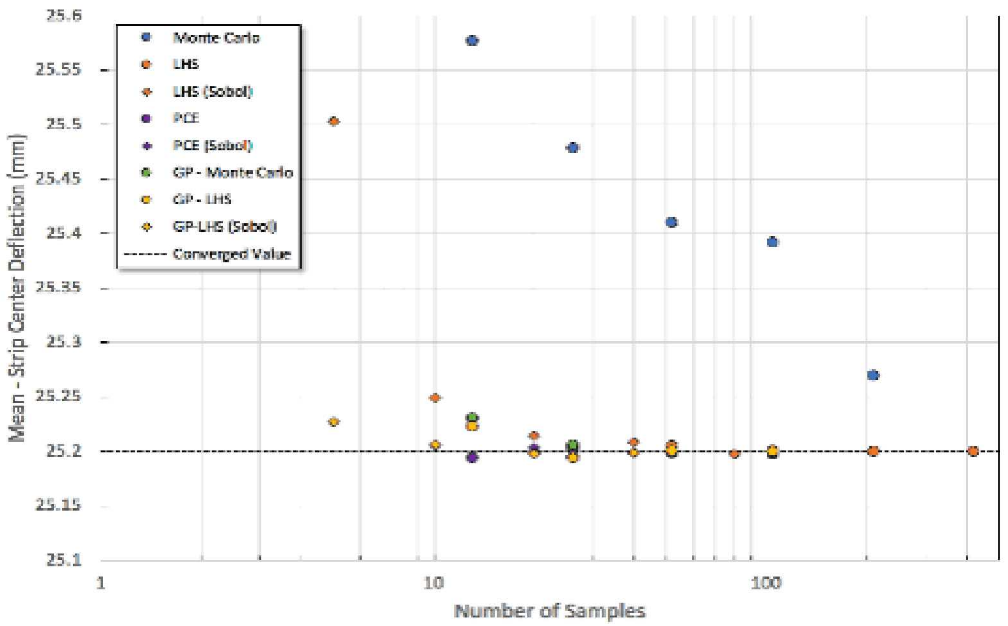
Summary of Sensitivity Study Survey

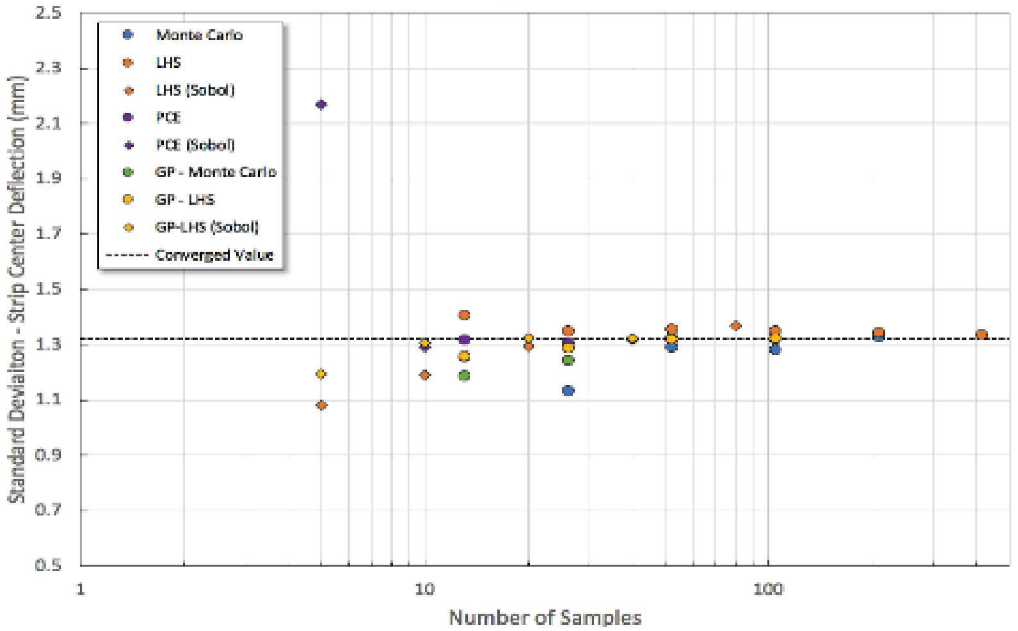
		Model Parameters																			
Method	Sample #	E_{11}	E_{22}	E_{33}	v_{12}	v_{13}	v_{23}	G_{12}	G_{13}	G_{23}	$\alpha_{11,G}$	$\alpha_{22,G}$	$\alpha_{33,G}$	$\alpha_{11,R}$	$\alpha_{22,R}$	$\alpha_{33,R}$	T_g	T_{st}	E_{Al}	v_{Al}	α_{Al}
CPS	41	■									■			■			■	■	■		■
	81	■	■								■			■			■	■	■		■
	121	■	■								■			■			■	■	■		■
MC	22	■	■	■	■	■	■		■	■	■	■	■	■	■	■	■	■	■	■	■
	44	■						■			■			■		■	■	■	■	■	■
	88	■	■								■			■			■	■	■		■
	176	■						■			■			■		■	■	■	■		■
	352	■						■			■			■			■	■	■		■
	704	■	■		■				■		■			■		■	■	■	■		■
	1408	■	■								■			■			■	■	■		■
	2816	■	■		■						■	■		■			■	■	■	■	■
	5632	■	■		■						■	■		■			■	■	■	■	■
LHS	22										■						■	■			■
	44	■	■							■	■			■			■	■	■		■
	88	■	■								■			■			■	■	■		■
	176	■	■								■			■			■	■	■	■	■
	352	■	■								■	■		■			■	■	■		■
	704	■	■		■						■			■			■	■	■	■	■
	1408	■	■		■						■	■		■			■	■	■	■	■
	2816	■	■		■						■	■		■			■	■	■	■	■
BBD	**761**	■	■		■						■	■		■			■	■	■		■
PCE	21	■	■			■			■		■			■			■	■	■		■
	42	■	■		■	■		■	■	■	■	■	■	■			■	■	■		■
	84	■	■								■	■		■			■	■	■	■	■
	168	■	■		■						■	■		■	■		■	■	■		■
	336	■	■		■						■	■		■	■		■	■	■	■	■
	672	■	■		■						■	■		■	■		■	■	■	■	■
GP	21				■		■					■	■	■		■					■
	42	■						■	■			■		■	■	■		■		■	■
	84	■	■	■	■	■	■	■	■	■	■	■	■	■		■	■	■	■		■
	168	■	■	■	■	■		■	■	■	■	■		■	■		■	■	■	■	
	336	■	■		■						■	■		■	■		■	■	■	■	■
	672	■	■		■						■	■		■	■		■	■	■	■	■

Comparison of UQ Methods

- Surrogate methods require the fewest samples for a converged mean prediction
  - Means converged at (n+1) samples
  - Standard deviations converge at 4(n+1) samples
- Sampling methods are the least efficient approaches
  - LHS requires 4x as many samples for a converged mean and >32x as many samples for a converged standard deviation
  - MC is not yet converged at 16x as many samples
- Converged predictions: 25.2 mm ± 1.32 mm
  - Prediction is within one standard deviation of measurement (26.41 ± 0.21 mm)!

Summary of UQ Methods Survey





Final Summary and Conclusions

- Residual stresses must be considered when designing composite parts
  - Finite element simulation of residual stresses are preferred to experimental measurement for complex structures
  - Sandia's process modeling approach has been well validated through collaboration with the AFRL
- A survey of DAKOTA's sensitivity and UQ capabilities was completed to find a validation procedure well suited to component qualification
  - What is the ideal sensitivity study approach?
    - Surrogates demonstrated the best computational efficiency
    - CPS should be used if a measure of sensitivity is needed for a expensive model
  - What is the ideal UQ approach?
    - Surrogates demonstrated the best computational efficiency
      - 4(n+1) samples appear to be sufficient for a surrogate converged for both mean and standard deviation predictions
  - Convergence must be checked!
- This approach can be applied generally when considering residual stress development in thin-walled composite structures

Thank you!

Back-Up

Parameter Study Method: Centered Parameter Study (CPS)

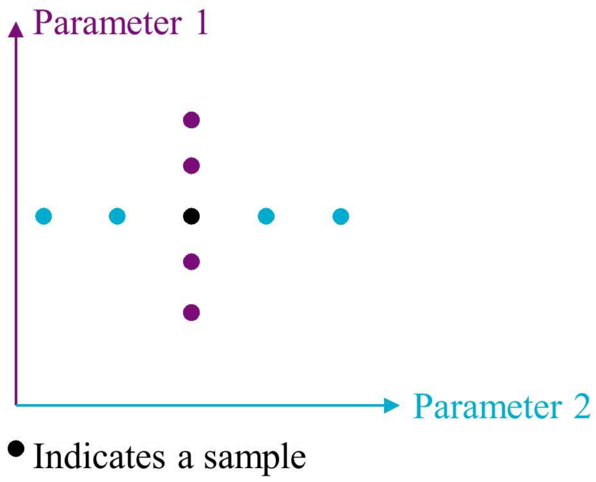
- One parameter study method was selected for consideration → CPS
  - DAKOTA also has multi-dimensional and vector parameter studies
  - CPS is cheapest, quantifies relationships between multiple model inputs and the simulated response
- General CPS approach: *"One-at-a-Time"*
  - Step 1: Define the parameter space and an initial value set
  - Step 2: Process a simulation with the initial value set
  - Step 3: For each parameter, process simulations at *s* steps ± the initial value. Values for all other model parameters held constant.
  - Step 4: Apply the ANOVA to the ensemble of predictions to determine the critical parameter list
- Bi-material strip CPS process:
  - Step 1: 20-dimensional parameter space, initial values defined by nominal properties
  - Step 2: Simulation processed with nominal material properties
  - Step 3: Starting with *s*=1 and step size= (max value – nominal value)/*s*, independently process simulations along each dimension.
  - Step 4: ANOVA applied to resulting 41 predictions to generate critical parameter list
  - Step 5: Repeat steps 3-4 with incrementally increasing *s* until critical parameter list is converged

Samples Required for CPS:

(n=dimensions, s=steps)

$$Samples_{CPS} = 1 + 2\sum_{i=1}^{s} n_s$$

Sample 2-Dimensional CPS Parameter Space



Design of Experiments: Box-Behnken Design (BBD)

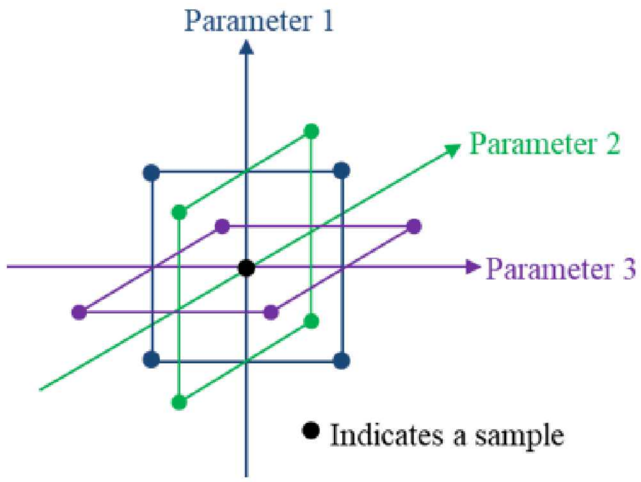
- One DOE method was selected for consideration → BBD
  - BBD does not sample outside of parameter space, requires fewer samples than other DOE methods
- General BBD approach:
  - Step 1: Define the parameter space with minimum, maximum, mean values
  - Step 2: Parameter combinations are created at the center and midpoints of the process space edges.
  - Step 3: A simulation is processed at each parameter combination
  - Step 4: Apply the ANOVA to the ensemble of predictions to determine the critical parameter list
- Bi-material strip BBD process:
  - Step 1: 20-dimensional parameter space
  - Step 2: BBD specified 761 parameter combinations
  - Step 3: 761 simulations were processed
  - Step 4: ANOVA applied to resulting 761 predictions to generate critical parameter list

Samples Required for BBD:

(k=number of parameters)

$$Samples_{BBD} = 1 + 2k(k-1)$$

Sample 3-Dimensional BBD Parameter Space



Sampling Methods: Monte Carlo (MC)

- Two sampling methods were considered → MC and LHS
  - MC is simple and easy to implement with any deterministic FE code
  - LHS is more complex, but provides better parameter space coverage with fewer samples

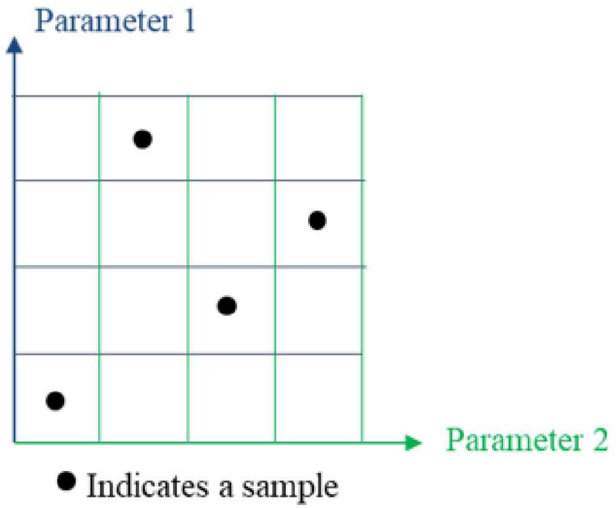
- Monte Carlo (MC)
  - Completely random sampling
    - No guarantee that any number of samples will cover parameter space
    - Convergence is assured, but a prohibitive number of samples may be required
  - General approach:
    - Step 1: Define the parameter space with minimum, maximum values
    - Step 2: Define the desired number of samples, N
    - Step 3: Process N simulations
    - Step 4: Apply the ANOVA to the N predictions to determine the critical parameter list
  - Bi-material strip MC process:
    - Step 1: 20-dimensional parameter space
    - Step 2: Initial samples size = 22, or $n+2$
    - Step 3: Process 22 simulations
    - Step 4: ANOVA applied to resulting 22 predictions to generate critical parameter list
    - Step 5: Repeat steps 2-4 with incrementally increasing N until critical parameter list is converged

Sampling Methods: Latin HyperCube Sampling (LHS)

- Latin HyperCube Sampling (LHS)
  - Stratified sampling technique
    - If N samples are desired, each parameter space dimension is divided into N segments of equal probability
      - Relative length of segments governed by probability distributions
    - N samples placed throughout parameter space grid → *One, and only one, sample can be placed in each bin*
      - Better coverage of parameter space!
  - General approach:
    - Step 1: Define the parameter space and probability distributions for each parameter
    - Step 2: Define the desired number of samples, N → Stratify parameter space
    - Step 3: Process N stratified simulations
    - Step 4: Apply the ANOVA to determine the critical parameter list
  - Bi-material strip LHS process:
    - Step 1: 20-dimensional parameter space, uniform distributions for all parameters
    - Step 2: Initial samples size = 22, or *n+2*
    - Step 3: Process 22 simulations
    - Step 4: ANOVA applied to resulting 22 predictions to generate critical parameter list
    - Step 5: Repeat steps 2-4 with incrementally increasing N until critical parameter list is converged

Sample 2-Dimensional LHS Parameter Space

(2 parameters and 4 samples)



Surrogate Methods: Polynomial Chaos Expansion (PCE)

- Two surrogate methods were considered → PCE and GP
- General surrogate model approach:
  - Minimally sample the parameter space to find a numerical function defining the relationship between the desired model output and the design variables
  - Sample the surrogate model 1000's of time at negligible cost
- Polynomial Chaos Expansion (PCE) → *Stochastic expansion method*
  - Multivariate orthogonal polynomials build the functional relationship between a response function and its random inputs
    - Polynomials are tailored to the specific input parameter distribution types → Legendre polynomial represent uniform distributions
  - Polynomial coefficients found through regression
    - LHS samples of the parameter space build a response function set that is fit with polynomials of varying order → Cross-validation determines best polynomial order

- General Approach:
  - Step 1: Define the parameter space and probability distributions for each parameter
  - Step 2: Define the desired number of LHS samples (*N*), stratify parameter space, process *N* stratified simulations
  - Step 4: Build the PCE surrogate using cross-validation to determine the best polynomial order
  - Step 5: Sample the surrogate model 1000's of times
  - Step 6: Apply the ANOVA to the surrogate samples to determine the critical parameter list

- Bi-Material Strip PCE process:
  - Step 1: 20-dimensional parameter space, uniform distributions for all parameters
  - Step 2: Initial samples size = 21, or $n+1$ → response function set size = 21
  - Step 4: PCE surrogate built considering polynomial orders 1-5
  - Step 5: 10000 samples were taken of the PCE surrogate
  - Step 6: ANOVA applied to resulting 10000 predictions to generate critical parameter list
  - Step 7: Repeat steps 2-6 with incrementally increasing *N* until critical parameter list is converged

Surrogate Methods: Gaussian Process (GP)

- Gaussian Process (GP)
  - All finite dimensional distributions must have a multivariate normal, or Gaussian, distribution
    - *Example*: Given a stochastic process, X, that is a function of the variables within a set T, for any choice of distinct values of T, the corresponding vector $\boldsymbol{X}$ must have a multivariate normal distribution
    - Normal distribution can be described by the finite dimensional distribution's mean and covariance functions → the Gaussian distribution is defined

- General Approach:
  - Step 1: Define the parameter space and probability distributions for each parameter
  - Step 2: Define the desired number of LHS samples (N), stratify parameter space, process N stratified simulations
  - Step 4: Assume response function set adheres to a Gaussian distribution and build the GP surrogate
  - Step 5: Sample the surrogate model 1000's of times
  - Step 6: Apply the ANOVA to the surrogate samples to determine the critical parameter list

- Bi-Material Strip GP process:
  - Step 1: 20-dimensional parameter space, uniform distributions for all parameters
  - Step 2: Initial samples size = 21, or $n+1$ → initial response function set size = 21
  - Step 4: GP surrogate was built
  - Step 5: 10000 samples were taken of the GP surrogate
  - Step 6: ANOVA applied to resulting 10000 predictions to generate critical parameter list
  - Step 7: Repeat steps 2-6 with incrementally increasing N until critical parameter list is converged

Material Parameter Criticality

- Summary of critical parameters:
  - All methods selected as critical: E_{11}, E_{22}, $\alpha_{11,G}$, $\alpha_{11,R}$, T_g, T_{sf}, E_{Al}, α_{Al}
    - In-plane mechanical/thermal properties of CFRP and aluminum properties should be critical
      - Residual stress development governed by in-plane CFRP/Al contraction mismatch
    - T_g and T_{sf} should be critical
      - T_{sf} indicates when residual stresses begin to develop
      - T_g governs rate of stress development
  - All methods, *except* CPS, selected as critical: ν_{12}, $\alpha_{22,G}$
  - All methods, *except* CPS and BBD, selected as critical: ν_{Al}
  - *Only* surrogate methods selected: $\alpha_{22,R}$
    - ν_{12}, $\alpha_{22,G}$, ν_{Al}, $\alpha_{22,R}$ may be less influential
- PCE surrogate can determine Sobol indices
  - Sensitivity indices → *rank critical parameters by relative influence*
  - Parameters selected by some, but not all, methods as critical of the lowest indices
  - The most significant indices govern the development of thermal strains
  - α_{Al} is most significant by a large margin
    - In-plane CTE of CFRP ≪ CTE of aluminum → aluminum thermal contractions drive residual stress development

PCE Sobol Indices

Parameter	Sobol Index
α_{Al}	98.003763%
T_{sf}	1.091548%
T_g	0.363556%
$\alpha_{11,G}$	0.354474%
E_{Al}	0.059520%
$\alpha_{11,R}$	0.056149%
E_{11}	0.027971%
E_{22}	0.001954%
ν_{12}	0.000305%
ν_{Al}	0.000301%
$\alpha_{22,G}$	0.000295%
$\alpha_{22,R}$	0.000018%
ν_{13}	0.000000%
E_{33}	0.000000%
$\alpha_{33,R}$	0.000000%
G_{23}	0.000000%
$\alpha_{33,G}$	0.000000%
ν_{23}	0.000000%
G_{13}	0.000000%
G_{12}	0.000000%