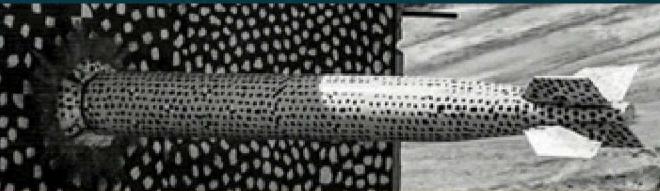


Survey of Sensitivity Analysis Methods During the Simulation of Residual Stresses in Simple Composite Structures



PRESENTED BY

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Presentation Outline

- Motivation and Objectives
- Validation Experiments
- Finite Element Methods
- Solution Verification and Mesh Optimization
- Sensitivity Study Methods Survey
- Discussion of Results and Conclusions
 - Ideal Sensitivity Study Methodology
 - Critical Parameters for Residual Stress Predictions

The background of the slide is a high-angle aerial photograph of a sprawling industrial or research facility. The complex is composed of numerous white and light-colored buildings, including large warehouses and smaller structures. It is situated in a valley, with a river or stream winding through the landscape to the west. The surrounding area is a mix of agricultural fields and green pastures, with rolling hills in the distance under a clear blue sky.

Introduction

Motivation

- Residual stresses should be considered when designing composite parts
- Computational simulation of process-induced stress state is an alternative to experimental measurements
 - Experimental approaches become impractical with increasing part complexity
- Sandia's simplified residual stress modeling approach has been validated
 - CTE mismatch and polymer shrinkage
 - Experimentally measured stress-free temperature
 - Requires the definition of 20+ material parameters
- Experimental characterization of many material properties not feasible
 - Sensitivity analysis methods can be employed to determine parameters critical to a simulated response
 - Critical parameters should be rigorously characterized, non-critical parameters can be approximated
- Many sensitivity analysis methods exist in the literature offering trade-offs between complexity and cost
 - Sampling methods are simple to implement, but computationally expensive
 - Surrogate methods are complex, but usually require fewer samples

- 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
 - Determine the ideal approach during the simulation of a composite's manufacturing process
 - Metric for comparison will be computational cost
 - Demonstrate how simulations can assist with allocating sparse experimental resources
 - Determine the material parameters most critical to predictions of a composite's process-induced stress state

The background of the slide is a high-angle aerial photograph of a sprawling industrial or research facility. The complex is composed of numerous white and light-colored buildings, including large laboratories and industrial structures. It is situated in a valley, with a winding river or stream visible in the foreground. The surrounding landscape is a mix of green fields, some with crops, and rolling hills in the distance under a clear sky.

Validation Experiment

Test Description

- Bi-material, CFRP/aluminum strip
 - Visually obvious post-fabrication residual stresses
 - Efficient and low-cost to model
- Dimensions:
 - In plane dimensions: 25.4 mm x 304.8 mm
 - Thickness: 1.6 mm (0.8 mm aluminum, 0.8 mm CFRP)
- Materials:
 - 8-harness satin weave, CFRP prepreg, $[0_2]_s$
 - Aluminum 6063-T6
 - Composite co-bonded to aluminum during an autoclave cure



- Process-induced stresses manifest as out-of-plane warpage/curling along the strip's length
 - CFRP and aluminum dissimilar CTE's
 - Irreversible strain due to polymer shrinkage
- Measurement procedure:
 - Granite table, guarantees flatness
 - Digital height gage, ± 0.01 mm
- One strip was manufactured and measured: 15.4 mm
 - Limited experimental rigor expended, sensitivity study survey not a validation exercise
 - Qualitative nature of the experiment indicates if the model captures the correct physical trends





Finite Element Methods



- Analysis Software:

- All simulations were processed with Sandia's SIERRA SolidMechanics/Implicit ("Adagio")
 - Lagrangian, three dimensional code for FEA of solid structures
 - Suitable for implicit, quasi-static analyses
- DAKOTA used to facilitate sensitivity study survey
 - Interface between SIERRA/SolidMechanics and iterative analysis methods
 - Available algorithms for sensitivity analysis, uncertainty quantification, and gradient and non-gradient based optimization

- Element Formulation:

- 8-noded hexahedral elements were used for all modeled components
- Adagio's default element formulation was used for simplicity and to reduce cost
 - Single point Gaussian quadrature
 - Hourglass modes are controlled through the definition of an hourglass stiffness

Material Models and Nominal Property Values

Aluminum 6063-T6

- Linear-elastic model (no yielding or failure expected)
 - Requires: density, Young's modulus, and Poisson's ratio
- Isotropic CTE
- Material properties taken from literature

Uncured CFRP

- Same linear-elastic model as aluminum
- Same Isotropic CTE as aluminum
- Material properties define a compliant and incompressible, isotropic-elastic solid
 - $E = 0.1 \text{ GPa}$, $\nu = 0.499$

Cured CFRP

- Linear-elastic orthotropic model
 - Requires: density, nine regular elastic constants, and material orientation
- Orthotropic CTE's
- Material properties taken from a combination of testing, micromechanical modeling, and literature

Nominal Aluminum Properties

Density, ρ (kg/m ³)	2,700
Young's Modulus, E (GPa)	68.9
Poisson's Ratio, ν	0.33
Coefficient of Thermal Expansion, CTE (1/°C)	23.4e-06

Uncured Composite Properties

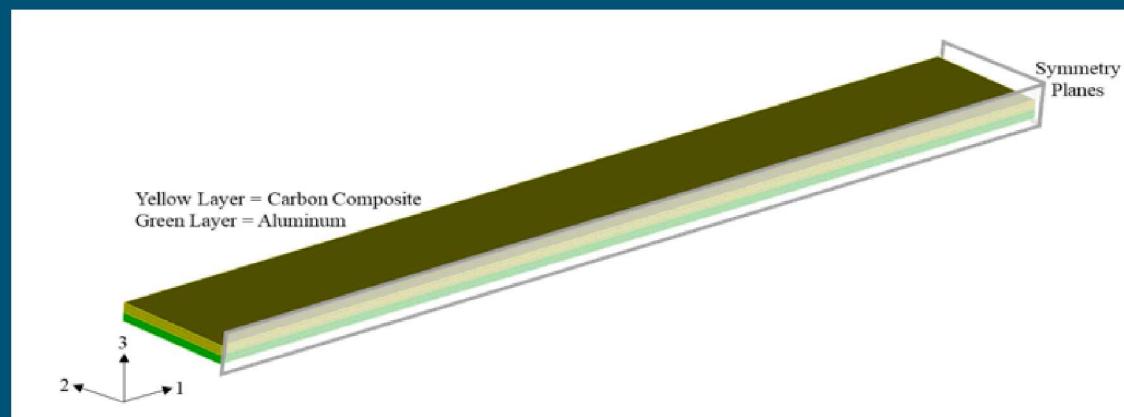
Density, ρ (kg/m ³)	1,600
Young's Modulus, E (GPa)	0.1
Poisson's Ratio, ν	0.499
Coefficient of Thermal Expansion, CTE (1/°C)	23.4e-06

Nominal Cured Composite Properties

Density, ρ (kg/m ³)	1,600	
Elastic Moduli, E_{11} , E_{22} , E_{33} (GPa)	63.86, 62.74, 8.59	
Poisson's Ratios, ν_{12} , ν_{13} , ν_{23}	0.0480, 0.4075, 0.0548	
Shear Moduli, G_{12} , G_{13} , G_{23} (GPa)	3.44, 3.27, 3.25	
Glass Transition Temperature, T_g (°C)	125.1	
Stress-Free Temperature, T_{sf} (°C)	143.3	
		Glassy Region Rubbery Region
Coefficient of Thermal Expansion, CTE ₁₁ (1/°C)	3.40e-06	1.13e-06
Coefficient of Thermal Expansion, CTE ₂₂ (1/°C)	3.36e-06	1.13e-06
Coefficient of Thermal Expansion, CTE ₃₃ (1/°C)	7.20e-05	2.83e-04

Model Geometry and Boundary Conditions

- Aluminum/CFRP modeled as separate, homogenized material layers
- CFRP layer merged to aluminum layer
 - Merging approximates perfect bonding, delamination is not modeled
- Boundary conditions:
 - Quarter model symmetry conditions assumed for computational efficiency
 - Two isothermal temperature cycles approximate the CFRP's curing:
 - Ambient (20°C) to stress-free temperature (143.3°C)
 - Stress-free temperature to ambient
 - CFRP's curing/stiffness change approximated with element activation



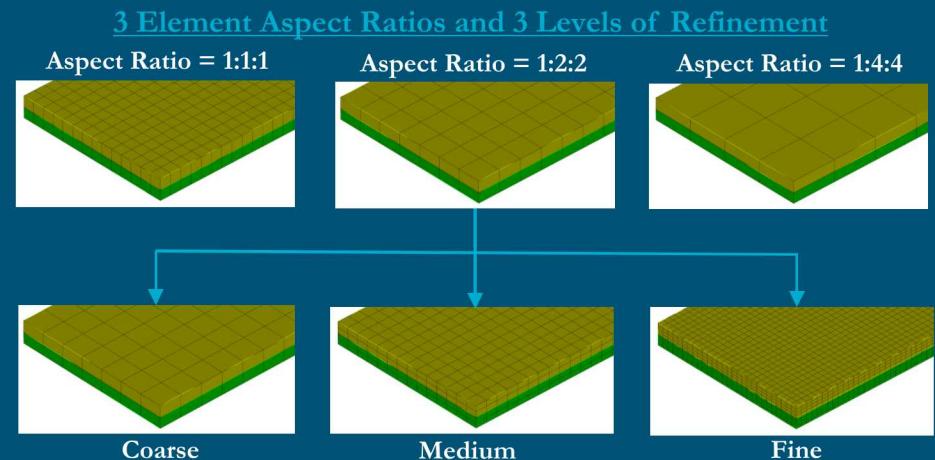
Element Activation

- CFRP's stiffness change due to the matrix material's polymerization reaction is approximated with Adagio's element activation
 - The stress/strain/deformation output of one simulation sets the initial stress/strain/deformation state of a subsequent simulation
 - An uncured composite material is simulated as compliant in one simulation and stiff in a subsequent simulation
- Bi-material strip processing modeled as two subsequent simulations:
 - Simulation #1:
 - Aluminum modeled as stiff, *CFRP modeled as compliant with uncured material properties*
 - Model is isothermally heated to stress-free temperature
 - Stress/strain/displacement data written to an output file
 - Simulation #2:
 - Input geometry, stress/strain/displacement states from output of simulation #1
 - CFRP assigned actual material properties (ACTIVATION)*
 - Model is isothermally cooled to room temperature, residual stresses form due to CTE mismatch

Simulation #	Components Modeled with <i>Actual</i> Material Properties	Components Modeled with <i>Compliant</i> Material Properties	Applied Temperature Boundary Conditions
1	Aluminum Layer	Composite Layer	Heating from 20°C to 143.3°C
2	Aluminum Layer, Composite Layer	None	Cooling from 143.3°C to 20°C

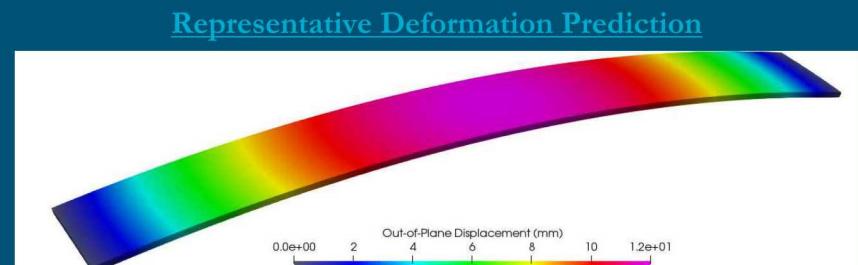
Solution Verification, Mesh Optimization, Nominal Model Validation

- Mesh study considered hex 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 FE 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



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	



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Sensitivity Analysis Methods

Survey Overview

- Sandia's residual stress modeling method requires the characterization of at least 20 parameters
 - Sparse experimental resources → Rigorous characterization not possible
 - Sensitivity analyses can assist in prioritizing/allocating experimental resources
 - Different methods offer trade-offs between complexity and efficiency
- Survey of DAKOTA's sensitivity analysis methods was completed with the verified bi-material strip model
 - What model parameters affect the residual stress predictions?
 - Which method is best for process modeling of composites?
- Six methods were examined:
 - Parameter study (centered parameter study)
 - Design of Experiments (Box-Behnken Design)
 - 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 \pm 3 standard deviations *or* \pm percentage of the nominal
 - Step 2: Complete sensitivity studies with the six methods
 - Step 3: Complete N-way ANOVA to find critical parameter list

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
Aluminum Properties	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
	E (GPa)	57.0	85.6
	ν	0.264	0.396
	CTE (1/°C)	18.7e-6	28.1e-6

Parameter Study Method: Centered Parameter Study (CPS)

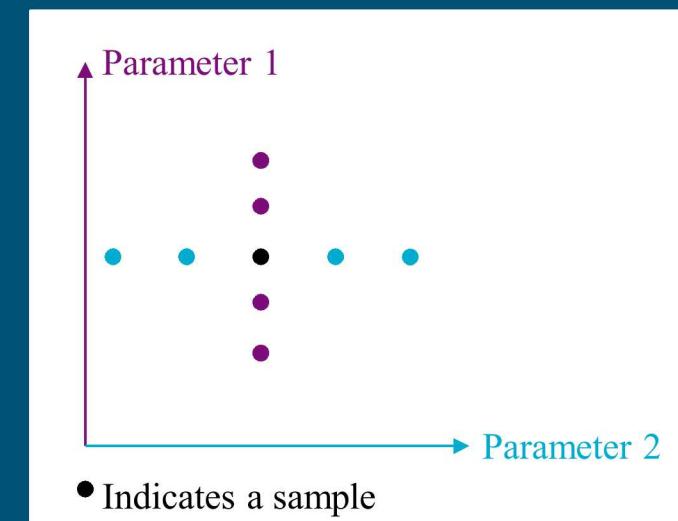
- One parameter study method was selected for consideration → CPS
 - DAKOTA also has multi-dimensional and vector parameter studies
 - CPS is cheapest, quantifies relationships between multiple model inputs and the simulated response
- General CPS approach: “One-at-a-Time”
 - Step 1: Define the parameter 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 \pm 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 = $(\text{max value} - \text{nominal value})/s$, 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:

($n = \text{dimensions}$, $s = \text{steps}$)

$$\text{Samples}_{CPS} = 1 + 2 \sum_{i=1}^s n_s$$

Sample 2-Dimensional CPS Parameter Space



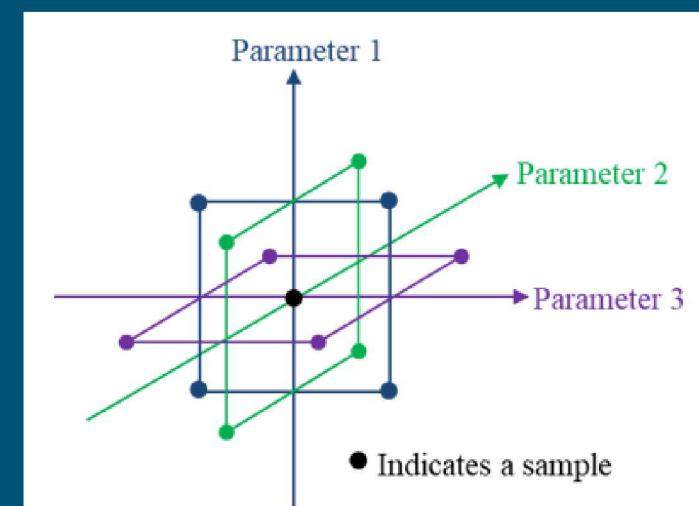
Design of Experiments: Box-Behnken Design (BBD)

- 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)

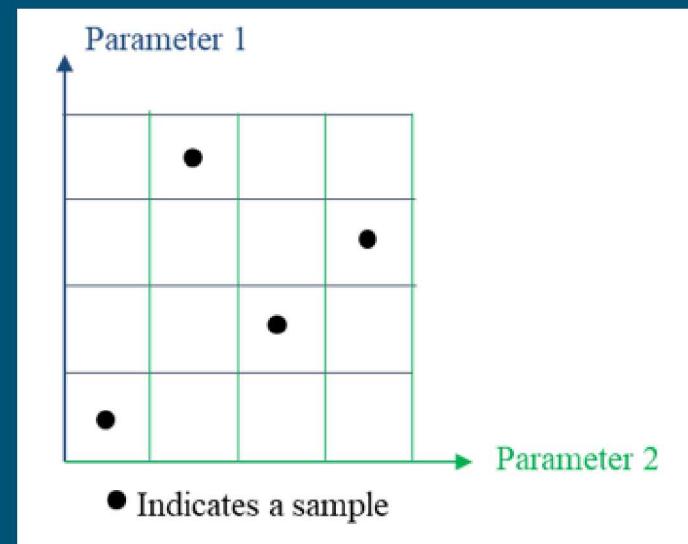
- Two sampling methods were considered → MC and LHS
 - MC is simple and easy to implement with any deterministic FE code
 - LHS is more complex, but provides better parameter space coverage with fewer samples
- Monte Carlo (MC)
 - Completely random sampling
 - No guarantee that any number of samples 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, $N \rightarrow$ 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 \mathbf{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 $n+1 \rightarrow$ 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

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Results and Conclusions



- Surrogate methods require the fewest samples for a converged list of critical parameters
 - GP may be preferred, slightly easier to implement
- Sampling methods are the least efficient approaches → 4-8x more expensive than surrogate methods
 - MC/LHS are simple to implement with any deterministic FE code
 - Merit consideration when lacking access to iterative analysis tools
- BBD is more efficient than the sampling methods, but twice as expensive as the surrogate methods
 - DOE methods are less complex than surrogates, can be implemented with any deterministic FE code
 - Should be considered as preferred alternative to sampling methods when lacking access to iterative analysis tools
- 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

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

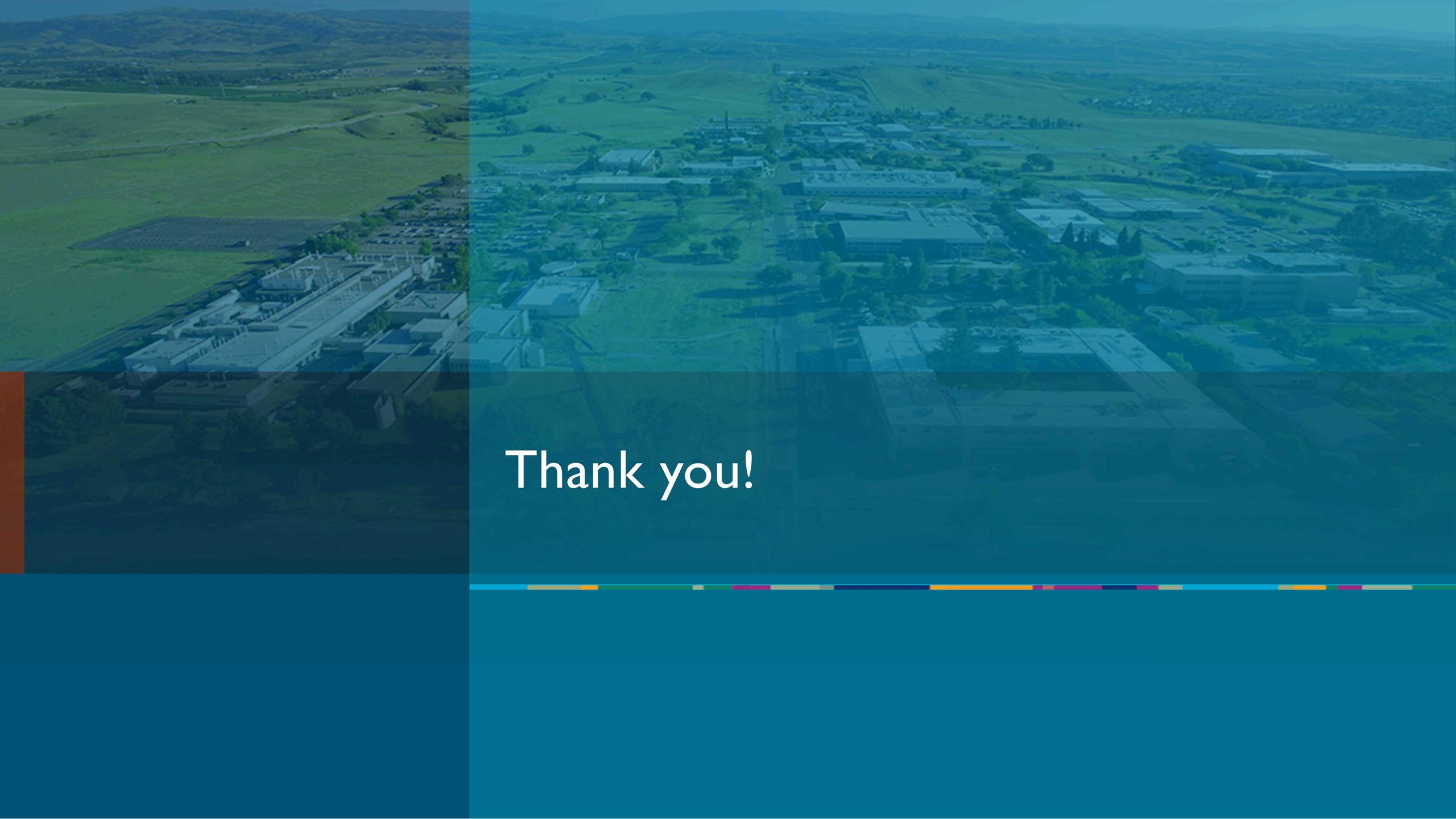
- Sensitivity indices → *rank critical parameters by relative influence*
- Parameters selected by some, but not all, methods as critical of the lowest indices
- The most significant indices govern the development of thermal strains
- α_{Al} is most significant by a large margin
 - In-plane CTE of CFRP ≪ 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%

Final Summary and Conclusions

- Residual stresses should be considered when designing composite parts
 - Finite element simulation of residual stresses may be preferred to experimental measurement
- Sandia's process modeling approach requires 20+ material parameters
 - Sparse experimental resources can make rigorous characterization impractical
 - Sensitivity surveys can be used to allocate experimental resources
- A survey of DAKOTA's sensitivity survey capabilities was completed with a process model of a mesh-optimized, bi-material CFRP/Aluminum strip
 - What is the ideal sensitivity study approach?
 - *GP/PCE* surrogates demonstrated the best computational efficiency
 - *BBD* approach should be used if there is no access to an iterative analysis toolkit
 - *CPS* should be used if parameter sensitivity is desired for an expensive model
 - Suggested methodology can be applied generally, not just to process modeling of composites
 - Which model parameters are most critical to a composite's residual stress predictions?
 - In-plane mechanical and thermal properties → in-plane contractions govern residual stress development at the bi-material interface
 - Stress-free and glass transition temperatures → T_g and T_{sf} govern when and with what rates residual stresses develop



Thank you!

