The Role of Uncertainty Quantification in Model Verification and Validation

Part 2
Model Verification and Validation Plan and Process
Case Study: Ni Superalloy Yield Strength Model

Dual Microstructure Disks

*Gabb et al., NASA Tech Report*

**Subsolvus**

**Supersolvus**

**Cooling Rates**

140 F/min to 338 F/min
Microstructure control through H.T. of disk superalloys

Temperature

~2000°F

Supersolvus

~1500°F, 8h

Subsolvus

Time

Subsolvus + fast cooling

primary γ′ + finer structure

Supersolvus + slow cooling

coarse structure
What is to be accomplished: Intended Use

- Verify model and input consistency based on given data
- Calibrate Anti-phase Boundary Energy (Apb0) and its temperature dependence (Qapb) using portions of LSHR subsolvus and supersolvus data sets
- Validate the calibrated model with remaining data.
  - Goal: Average of less than 3% difference in predicted Yield Strength as compared to experimental results across temperature range
- Perform global sensitivity analysis of validated model to guide future experimental efforts.
V&V Process

- Design and develop models
- Verify the model implementation
- Perform UQ and sensitivity studies to understand uncertainties
- Design validation/calibration experiments
- Perform experiments
- Assess accuracy (validation)
- Revise model/experiment
- Document the model, process, and accuracy assessments
V&V Plan

- Driven by customer
- Model description
  - Intended use of the model
  - Conceptual model
  - Mathematical model
  - Input parameters
  - Design space domain
  - System response quantities
  - Model/Validation hierarchy
  - Phenomena identification and ranking technique (PIRT)
- Verification approach
- Validation experiments
- Validation metrics and requirements
- Cost and schedule constraints
- Programmatic assumptions and limitations
Conceptual Model – Collection of assumptions and descriptions of physical processes representing the behavior of the reality of interest from which the mathematical model and validation experiments can be constructed.
Conceptual Model: Case Study

- Intended use of the model is to predict the yield strength as a function of temperature, microstructure, and heat treatment.
- Design space domain documents the range of environments, dimensions, chemistry, etc. that are relevant to the intended use of the model.
  - LSHR Nickel superalloy using two separate heat treatments (sub- and supersolvus)
  - Temperature range: 70-1500F.
Mathematical Model

- Mathematical Model – Mathematical equations, boundary values, initial conditions, and modeling data needed to describe the conceptual model.

\[
\left[ EI(x)y'' \right]'' = w(x) \quad 0 < x < L \\
y(0) = y'(0) = y''(L) = y'''(L) = 0
\]
Mathematical Model: Case Study

- Mathematical Model – proprietary Excel model
Computational Model

- Computational Model – Numerical implementation of the mathematical model, usually in the form of numerical discretization, solution algorithm, and convergence criteria.
Validation Hierarchy

- **Validation hierarchy**
  - Breaks the problem into smaller parts
  - Validation process employed for every element in the hierarchy (ideally)
  - Allows the model to be challenged (and proven) step by step
  - Dramatically increases likelihood of right answer for the right reason

- **Customer establishes intended use and top-level validation requirement**

- **Validation team constructs hierarchy, establishes sub-level metrics and validation requirements**

- **In general, validation requirements will be increasingly more stringent in lower levels**
  - Full system sensitivity analysis can provide guidance
Model Hierarchy

Yield strength, $\sigma_y(T)$

Critical resolved shear stress (CRSS)

- APB
- Coherency
- Volume fraction
- Precipitate size
- Matrix friction stress
- Precipitate friction stress

Inputs

- Temperature
- Primary $\gamma'$ size
- Primary $\gamma'$ $V_f$
- Secondary $\gamma'$ size
- Secondary $\gamma'$ $V_f$
- APB Energy
- APB Temp. Dep.
PIRT

- Relevant physical processes to predict the reality of interest
- Key elements and technical issues in both the conceptual and computational models.
- Captures relevant phenomena and simplifying assumptions
- Describe potential technical issues and barriers
- Ranks relative importance of these issues
- Resource allocation
- Communication
- Supports V&V plan and the UQ strategy
## Model PIRT

<table>
<thead>
<tr>
<th></th>
<th>Type</th>
<th>Importance</th>
<th>Confidence</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>A.1</td>
<td>Microstructure</td>
<td>High</td>
<td>Medium</td>
<td>Small errors in the tertiary γ’ volume fraction and size lead to large errors in yield strength</td>
</tr>
<tr>
<td>A.2</td>
<td>Chemistry</td>
<td>High</td>
<td>High</td>
<td>Generally well characterized</td>
</tr>
<tr>
<td>B.1</td>
<td>Grain size hardening</td>
<td>High</td>
<td>Medium</td>
<td>Strengthening inversely proportional to grain size, doesn’t apply to single crystal systems</td>
</tr>
<tr>
<td>C.1</td>
<td>Matrix Friction</td>
<td>Medium</td>
<td>Medium</td>
<td>Chemistry/Temp effect. Form is a fit to literature data per material composition</td>
</tr>
<tr>
<td>C.2</td>
<td>Precipitate Friction</td>
<td>Medium</td>
<td>Medium</td>
<td>Solution strengthening effect</td>
</tr>
<tr>
<td>D.2</td>
<td>Interface Strengthening</td>
<td>High</td>
<td>Medium</td>
<td>Includes APB effects, coherency strain</td>
</tr>
</tbody>
</table>
## Input Parameter PIRT

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<td>High</td>
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<td><strong>PySiz</strong></td>
<td>Primary $\gamma'$ size</td>
<td>High</td>
<td>Medium</td>
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<td><strong>PyVf</strong></td>
<td>Primary $\gamma'$ $V_f$</td>
<td>Medium</td>
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<td><strong>APB0</strong></td>
<td>Anti-phase boundary energy</td>
<td>High</td>
<td>Low</td>
</tr>
<tr>
<td><strong>QAPB</strong></td>
<td>Anti-phase boundary energy temperature dependence</td>
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## Experiment PIRT

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<th>UQ Mitigation</th>
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<tr>
<td>A.1</td>
<td>Force application/measurement</td>
<td>High</td>
<td>High</td>
<td>Measurement tolerances provided by supplier</td>
</tr>
<tr>
<td>A.2</td>
<td>Displacement measurement</td>
<td>High</td>
<td>High</td>
<td>Measurement tolerances provided by supplier</td>
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<tr>
<td>A.3</td>
<td>Temperature application/measurement</td>
<td>High</td>
<td>Medium</td>
<td>Measurement tolerances provided by supplier</td>
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<tr>
<td>B.1</td>
<td>Specimen geometry</td>
<td>High</td>
<td>High</td>
<td>Measure specimen geometry</td>
</tr>
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<td>C.1</td>
<td>Stress-strain conversion</td>
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<td>Medium</td>
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Verification

- Verification: The process of determining that a computational model accurately represents the underlying mathematical model and its solution.
  - Code Verification – establish confidence, through the collection of evidence, that the mathematical model and solution algorithms are working correctly.
    - What? Code Solution = Analytical Solution?
    - Who? Developers & Users
  - Calculation Verification - establish confidence, through the collection of evidence, that the discrete solution of the mathematical model is accurate.
    - What? Discretization Error
    - Who? Developers & Users
Verification Approaches

- Analytical solutions or benchmarks
- Engineering approaches
- Ranges defined by the design space domain
  - LSHR Nickel superalloy (sub- and supersolvus)
  - Temperature range: 70-1500°F
- Documentation
Verification: Case Study

- No analytical solutions
- Trends understood
- Exercised model over design space domain
Quantification of random and epistemic uncertainties in both model and test
Uncertainty Propagation

Material Properties

Loadings

Boundary Conditions

Response and Failure Model(s)

Bounds due to model uncertainty

Reliability

Service Life

Life

Probabilistic Sensitivity Factor

Location Radius Load S-N Scatter
Uncertainty Quantification

- Calibration parameters (APB0, QAPB)
- Measured microstructure
- Measured yield strength
- Ranges defined by the design space domain
  - LSHR Nickel superalloy (sub- and supersolvus)
  - Temperature range: 70-1500F

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The validation process has the goal of assessing the predictive capability of the model by comparing the predictive results of the model with validation experiments.

Three key elements of Validation:
- Validation Experiments
- Uncertainty Quantification
- Validation Metrics
Validation/Calibration Experiments

- Calibration experiments to define key model inputs (APB0, QAPB)
- Validation experiments to determine model accuracy
- Ranges defined by the design space domain
  - LSHR Nickel superalloy (sub- and supersolvus)
  - Temperature range: 70-1500F

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Validation: Case Study

- Select metrics
  - Repeat experiments
  - Experiments over range of control variable
- Ranges defined by the design space domain
  - LSHR Nickel superalloy (sub- and supersolvus)
  - Temperature range: 70-1500F
Initial Model Development

- Use the PIRT to guide sensitivity studies for phenomena or variables where importance/confidence may not be known well
  - Exercise the initial model to see if model development or experiments need to be performed
  - Could be “missing” physics but some value is usually gained
- Use the model hierarchy to develop verification strategies
  - Are there cases where we can exercise the model through key elements in the hierarchy with known solutions?
V&V Plan is a Working Document

- Model hierarchy and PIRTs guide
  - Uncertainty quantification
  - Verification
  - Validation experiments
  - Resource allocation
- PIRTs are usually updated as more is learned during the process
- Validation and UQ strategies may change as more is learned