



Computational Materials for Qualification and Certification of Process-Intensive Metallic Materials (CM4QC): Navigating the Valley of Death

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E.H. Glaessgen

*NASA Senior Technologist for Computational Materials
NASA Langley Research Center*

and

Michael Gorelik

*FAA Chief Scientist and Technical Advisor
for Fatigue and Damage Tolerance*

Approved for Public Release on
Case Number:



Legal Statements



The purpose of this group is not to establish Federal policy, but to enable a free-ranging discussion of emerging issues. Participants have provided non-consensus, non-voting advice, informational background, and technical and administrative assistance.

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The views expressed in this document are those of the authors themselves and do not necessarily represent the views of their individual institutions.

- Evolution of Complexity and Use of Additively Manufactured (AM) Parts
- Computational Materials Landscape
- Some Regulatory Constraints & Opportunities from FAA
- CM4QC Steering Group, Goals, Membership and Operation
- Highlights of the CM4QC Roadmap
- Elements of the CM4QC Steering Group's Phase II Plan
- Summary

Increasing Complexity of AM Parts

Configuration, Application, Composition/Microstructure

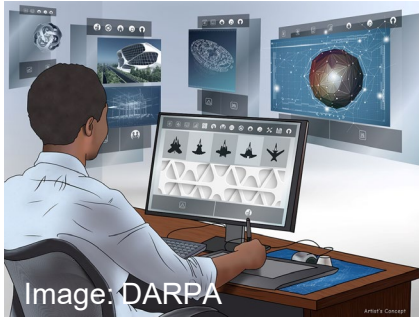
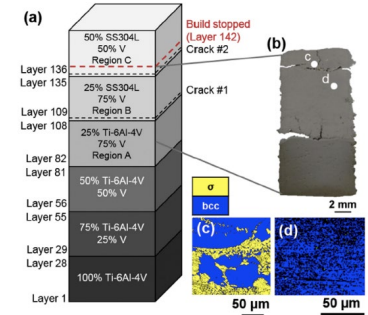
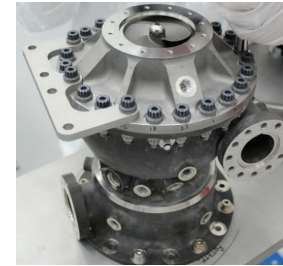


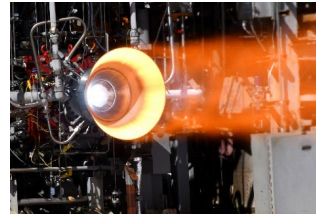
Image: DARPA
DARPA TRADES* Program



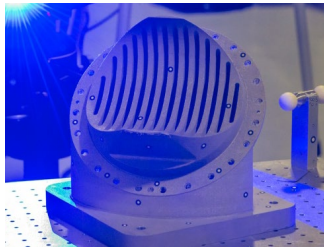
Graded Materials
Image: NASA**



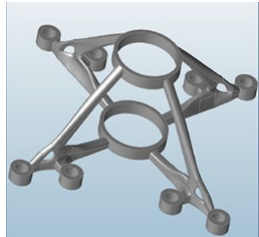
Turbopump Housing
Image: NASA



Rocket Engine Nozzle
Image: NASA



Pogo Z-Baffle
Image: NASA



Bracket
Image: NASA

Increasing Complexity

* TRANSformative DESIGN

Bobbio *et al.* (2018) *J. Alloys and Compounds*, **742 1031

AM Offers Unprecedented Potential (e.g., DARPA TRADES Program*)



Transform design by exploring new math/algorithms to:

- Harness the tidal wave of new materials and fabrication methods coming our way and enable new designs that are unimaginable today.

Vision

- Advance the foundational mathematics and computational tools required to generate and better manage the enormous complexity of design.
- TRADES intends to develop engineering tools to address design representation, analysis, and synthesis.

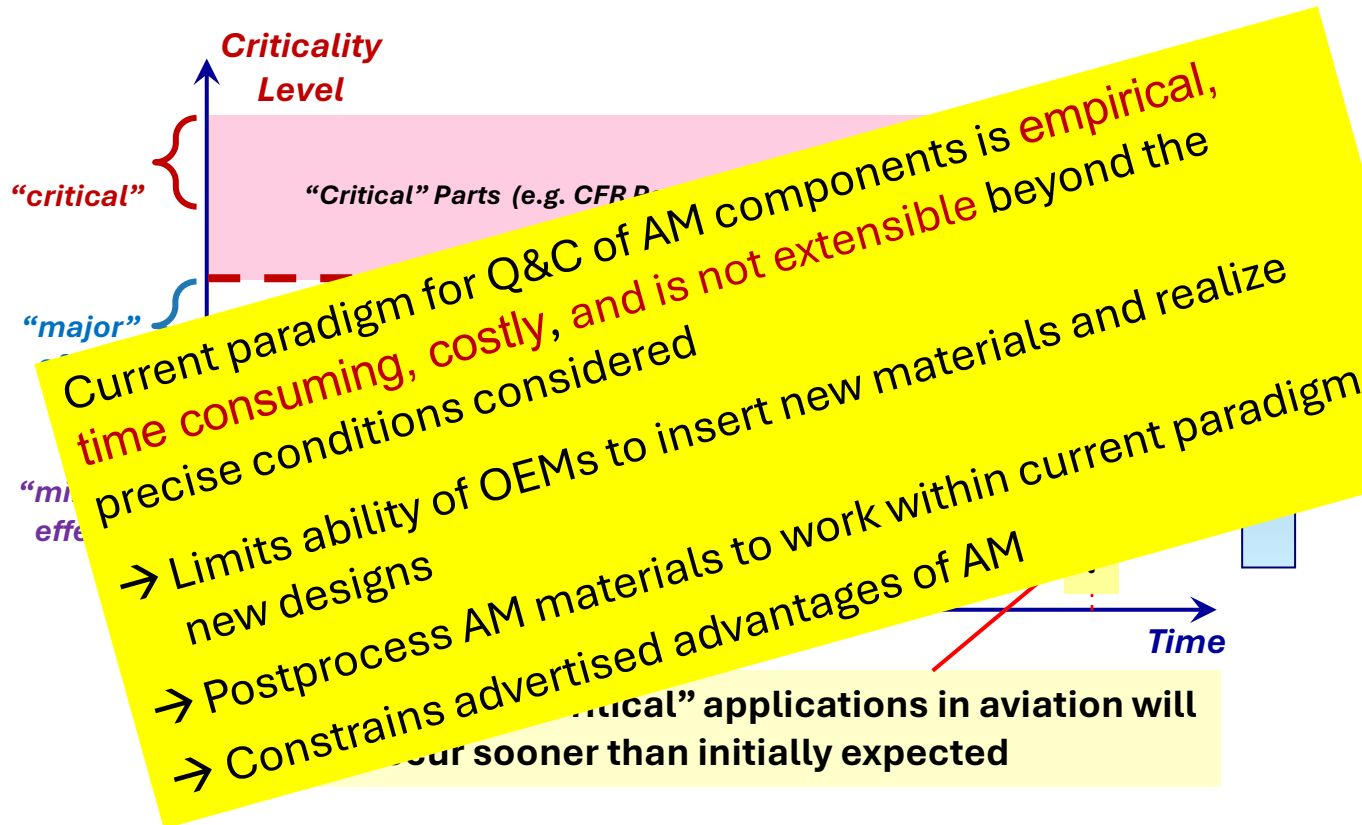
Goals

- TRADES technologies will allow designers to more easily navigate the design space to discover non-intuitive yet realizable designs that **fully leverage new materials and advanced manufacturing approaches**, ultimately showing a way forward for future design systems and processes.



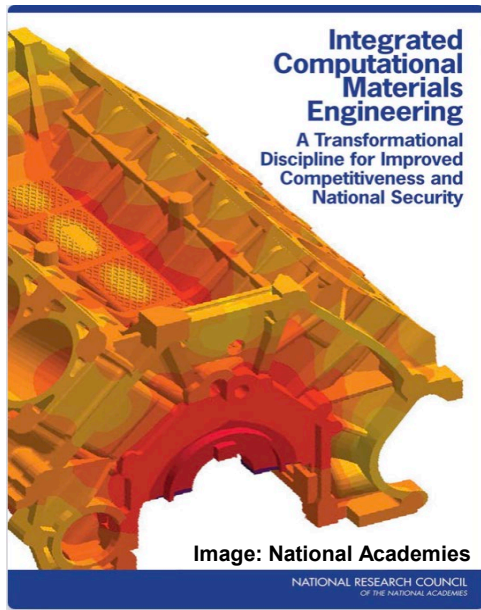
* Jan Vandenbrande, DARPA/DSO

Evolution of Criticality of AM Parts



- CFR - Code of Federal Regulations
- PSE – Principal Structural Element
- LLP – Life Limited Part
- Q&C – Qualification and Certification
- AM – additive manufacturing
- OEM – original equipment manufacturer

Computational Materials Landscape



2008



2011

- Computational Materials and Data Science approaches to design new materials with new functionalities...Faster
- Material Qualification practices are substantially the same as they have been for decades

→ Currently, maturation through TRL*-scale from laboratory coupons to flight-qualified materials (and flight-certified parts) does not benefit from these technologies

“Make It and Break It” Q&C Testing Practices



- Will they become extinct anytime soon...no
- Can we improve upon themyes

➡ using Computational Materials-informed Approaches

What does the FAA mean by Qualification & Certification



Qualification

- Demonstration that the **manufacturing process, feedstock material, etc** produces a structural material that is repeatable and meets requirements of interest (e.g., fatigue life)
- Main focus is on **qualifying material or manufacturing process**, and is typically performed by a company (“applicant”) prior to starting a formal certification process

Certification

- A process of showing compliance with **regulatory requirements** for a product (e.g., an aircraft) or a specific structure
- The **structure** performs as intended (typically includes material and manufacturing qualification data)

- **Requirements for Certification are Public Information**
- **“Means of Compliance” could be either OEM’s Intellectual Property, or public information (e.g. FAA guidance materials, public standards)**
→ **Data generated to show compliance is typically OEM-proprietary**

Examples of “Model-Friendly” Domains



In the Context of FAA Regulations – Title 14 CFR Parts 25 (Airframe) and 33 (Engines)

- Damage Tolerance → Part 25 (AC 25.571-1D)
In general, “analysis supported by test evidence” is accepted



- Damage Tolerance → Part 33 (AC 33.70-1)
Analysis is accepted (e.g., stress, heat transfer, crack growth, ...)
However, “...the analysis approach should be validated against relevant test data”



Fall 2019

- Visit by M. Gorelik (FAA Chief Scientist for Fatigue and Damage Tolerance)
- Discussion Topic: Limitations of current approaches for Q&C and potential improvements
- The Possibility Space: Development, maturation (including V&V/UQ*), regulatory acceptance and industrial use of Computational Materials-informed Q&C approaches

January 2020

- Industry, Government, University workshop at Langley
- Recommendation to create...
CM4QC Steering Group

NASA/TM-20210015175

DOT/FAA/TC-20/38



NASA / NIST / FAA Technical Interchange Meeting on
Computational Materials Approaches for Qualification by
Analysis for Aerospace Applications

Edward H. Glaessgen
Langley Research Center, Hampton, Virginia

Lyle E. Levine, Paul W. Witherell, and M. Alkan Donmez
National Institute of Standards and Technology, Gaithersburg, Maryland

Michael Gorelik
Federal Aviation Administration, Scottsdale, Arizona

Nathan A. Ashmore
Boeing Research and Technology, St. Louis, Missouri

Richard R. Barto
Lockheed Martin Advanced Technology Laboratories, Cherry Hill, New Jersey

Corbett C. Battaile
Sandia National Laboratory, Albuquerque, New Mexico

Harry R. Millwater
University of Texas at San Antonio, San Antonio, Texas

Gerard J. Nanni
Bell, Fort Worth, Texas

Anthony D. Rollett
Carnegie Mellon University, Pittsburgh, Pennsylvania

Edwin J. Schwalbach
Air Force Research Laboratory, Dayton, Ohio

Vasisht Venkatesh
Pratt and Whitney, East Hartford, Connecticut

May 2021

*V&V/UQ: Verification & Validation /
Uncertainty Qualification

Computational Materials for Qualification and Certification (CM⁴QC) Steering Group



The ***primary goals*** of this Steering Group are to

- Provide **coordination for and focus to investments** made by U.S. industry and the U.S. government toward development of computational materials-based approaches for Q&C of process-intensive metallic materials.
- Identify key considerations and enablers required to **increase airworthiness / certifying authorities' acceptance of CM methods** used for Q&C of structural or flight-critical process-intensive material (PIM) parts.
- **Increase dialogue** among the stakeholder organizations and seek opportunities for coordination & collaboration.

Membership includes subject matter experts from the aerospace industry, regulatory authorities, various government laboratories and academia

Steering Group Membership

Make Business Case → Define Needs → Plot Path Forward → Provide Unified Vision

Government

National Aeronautics and
 Space Administration
 Federal Aviation
 Administration
 National Institute of
 Standards and Technology
 Sandia National Laboratory
 U.S. Air Force Research
 Laboratory
 U.S. Army Aviation Command
 U.S. Navy Air Systems
 Command
 Oak Ridge National
 Laboratory

Industry

The Boeing Company
 Lockheed Martin
 Raytheon / Pratt &
 Whitney
 General Electric Aviation
 Spirit Aerosystems
 Honeywell Aerospace
 Southwest Research
 Institute
 Northrop Grumman
 Textron Aviation

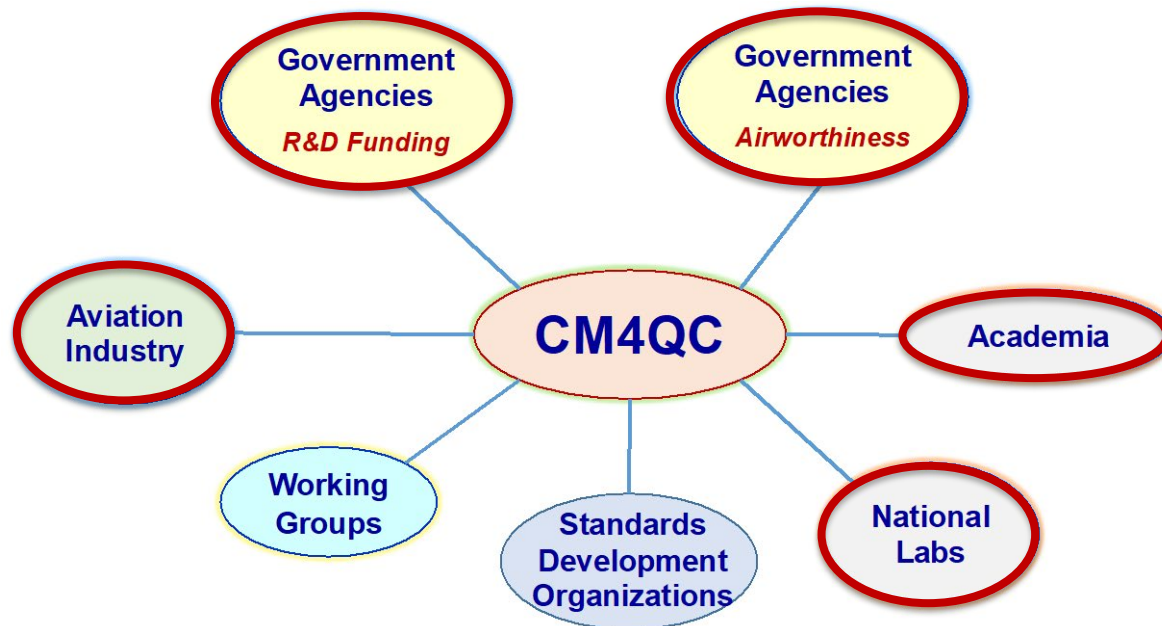
Academia

Univ Texas San
 Antonio
 Carnegie Mellon Univ.
 Vanderbilt Univ.
 Pennsylvania State
 Univ.
 Northwestern Univ.

Operation of the CM⁴QC Steering Group



- **Working Group 1: Understanding industry** priorities / timeline and key regulatory implications (High TRL*)
- **Working Group 2: Strategies for maturation and transition** of Research to Engineering (Mid TRL, Valley of Death)
- **Working Group 3: Development of required** computational materials and measurement **capabilities** (Low TRL)



**Initial outcome –
Multi-year implementation plan**

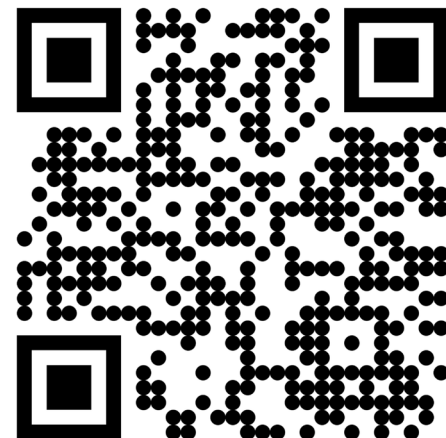


NASA/TM-20260001729

DOT/FAA/TC-26/10

CM4QC Website

[https://www.nist.gov/
programs-projects/cm4qc](https://www.nist.gov/programs-projects/cm4qc)



Sections 1-3: Introductory Material

Section 1: Background

Examples:

- The Problem
- Prior Related Government Efforts
- Current Uses of Computational Materials
- Importance of VV / UQ

Section 2: Scope

Examples:

- Key Objectives
- Desired Impacts
- Gaps Limiting Maturation and Adoption

Section 3: Industry's Vision for Q&C of AM

Examples:

- *Q&C decisions based on performance risk*
- Lower barriers to insertion of new materials and new configurations
 - *The ability to fly designer materials (e.g., computanium)*

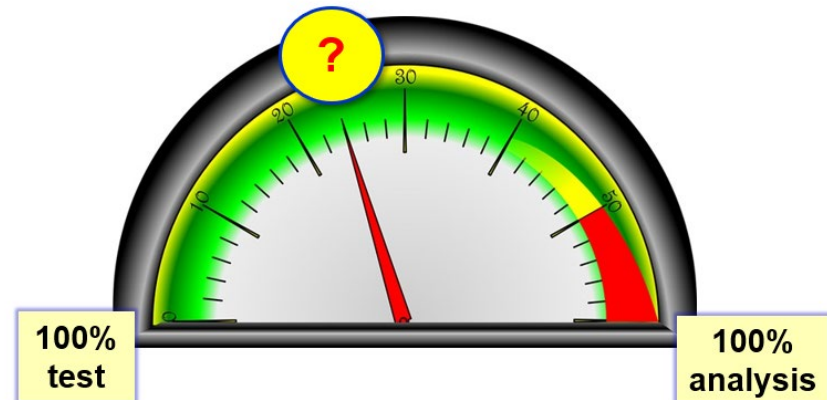
Section 4: Regulatory Considerations for Acceptance of Computational Materials-informed Q&C



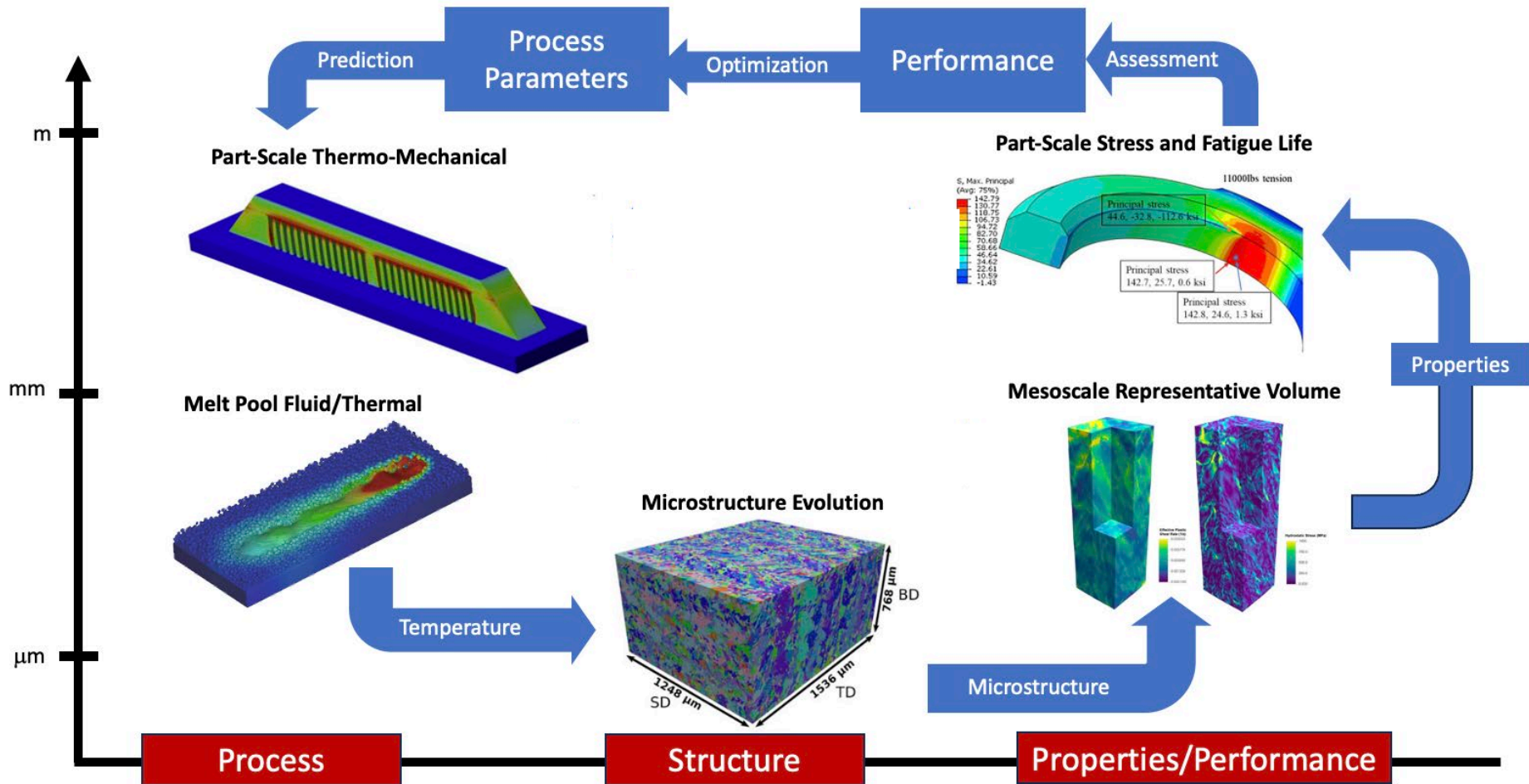
Key drivers

- Gradual **reduction in conventional Q&C test matrices**
- **Optimization of material test matrices** informed by CM insights (i.e., obtaining the most valuable information from testing)
- Exploring the corners and fringes of the multi-dimensional process parameter space to **fully capture material performance variations**
- Understanding **process limitations and potential failure modes**
- Better understanding of the similitude (or a lack thereof) between the performance of the **test specimens vs. parts**

***Future State: Balance
between Test Data
and
CM-informed Q&C is
Undetermined***



Section 5: Key Computational Materials Capabilities & Enabling Technologies



**Process Structure Property/Performance
(PSP/P) Modeling Framework**

Section 6: Key Elements & Associated Methods for CM Verification, Validation & Uncertainty Quantification



Focus of text below is on Validation Metrics

- Validation metrics should be **quantitative and objective**
- Criteria used by an analyst/designer to accept a model for prediction should be **separate from the validation metric** itself
- **Uncertainties** resulting from **both computer models and experiments** should be considered
- Validation metrics should provide a **statistical confidence level** associated with the amount of available experimental data
- Validation metrics should also differentiate between models containing greater and lesser **amounts of uncertainty**
- A metric should have the flexibility of **measuring the agreement of prediction and physical observations** either at a single setting or multiple settings of controllable inputs over an intended prediction region to assess the global predictive capability.

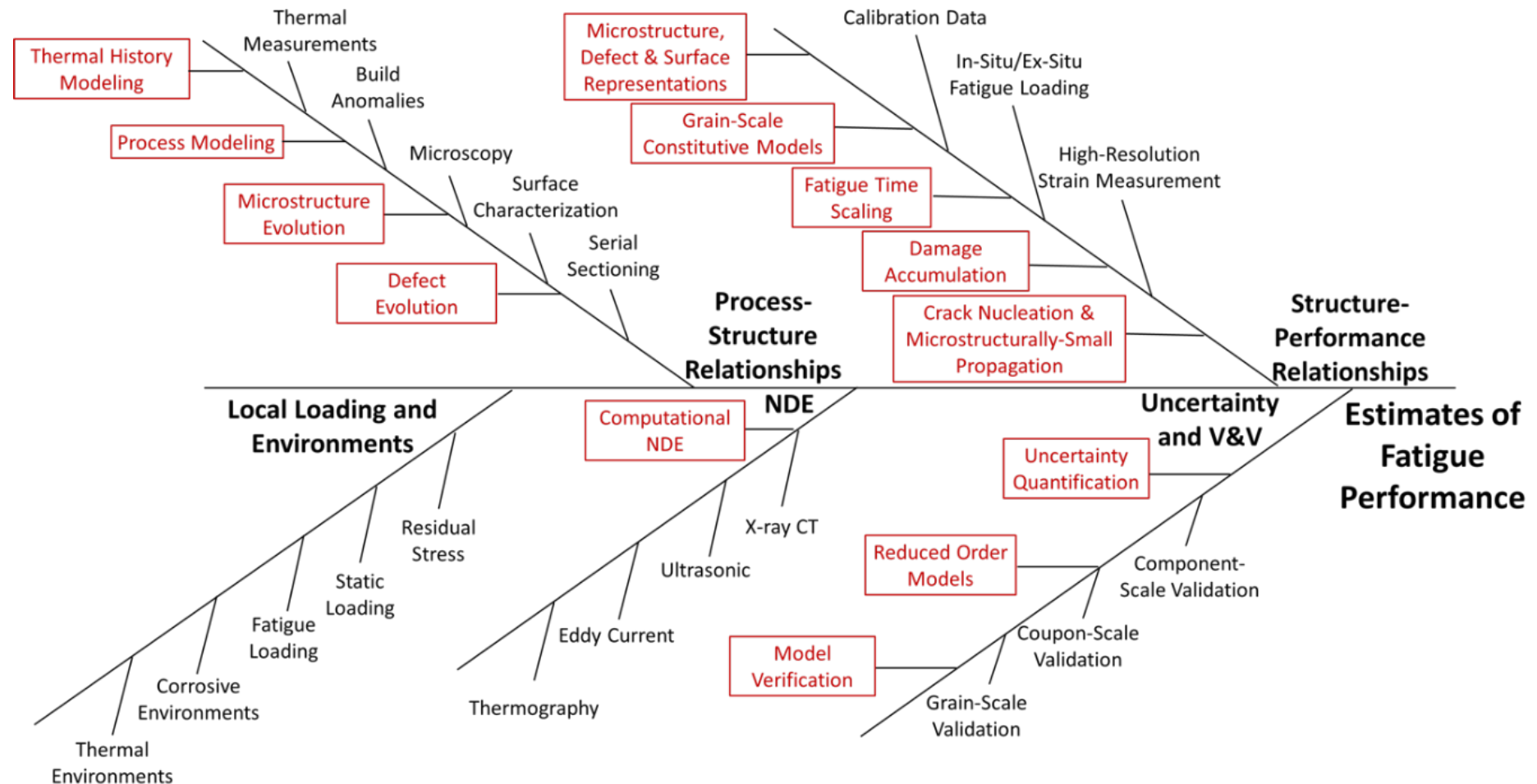
Section 7: CM Simulation Maturity Level (SML) Assessment Framework*



Maturity Level	Description
1	All underlying models are clearly defined, including inputs, outputs, and application intent. Analytical process is exploratory in nature. Fidelity of predictions is largely unproven. Provides some physical insight, but not yet suitable for adoption in Q&C activities.
2	Proven capability for comparative assessment, ranking, or trending. Experimental validation remains incomplete. Can be used to inform other activities relevant to Q&C.
3	Capability is verified and validated for limited cases. Use is primarily limited to research activities. Impact to industry activities occurs primarily through work where results could be used to inform Q&C activities.
4	Capability is fully verified and validated for industry use cases. Simulation platform is used by industry, but relevance is primarily to research activities, with occasional direct impact to Q&C activities. Results are used primarily to provide guidance and confidence to design and development activities.
5	Simulation platform is widely adopted by industry. Model predictions are directly applicable to Q&C activities.

*Adapted from: B. Cowles, D. Backman, R. Dutton, "Verification and validation of ICME methods and models for aerospace applications," Integrating Materials and Manufacturing Innovation, vol. 1 (2012), pp. 3–18.

Section 8: Technology Maturation Path



Fishbone diagram showing inputs and dependencies that contribute to Estimates of Fatigue Performance

Section 9: R&D Investment Opportunities for Computational Materials in the Q&C Domain



Example: Properties and Performance

	Topic	Status	Tractability
Physics: Properties and Performance	22. Static mechanical properties (YS, work hardening)		
	23. Static mechanical properties (ductility, ultimate tensile strength (UTS))		
	24. Creep		
	25. Fatigue life (initiation and short crack growth)		
	26. Fatigue life (long crack growth)		
	27. Fracture toughness		
	28. Environmental effects		
	29. Part scale geometric effects		

Section 10: Computational Materials Ecosystem Maturation Path (1 of 3)



How Can CM **Augment (Rather than Replace)** Existing Q&C practices?

- Investment in CM capability development
- Transition to next-generation AM machines to enable CM-informed Q&C
- ➔ Characterization and data practices for calibration, validation, and machine learning
- ➔ CM4QC culture
 - Development of AM-appropriate regulatory standards
 - CM education and workforce development

Characterization and Data Practices for Calibration, Validation and Machine Learning

Calibration Data Include

- Material Properties of Molten Materials (Coefficient of Thermal Expansion, Specific Heat, Surface Tension, Viscosity, ...)
- Process Parameters (Scan Path, Layer Height, Laser Power, ...)
- Microstructure Characteristics (Solid/Liquid Surface Energy, Nucleation Density Solid-Solid, ...)
- Material Properties of Solid Materials (Dislocation Density, Grain Size, Precipitate Size, Defect Distributions, ...)

Validation Data Include

- Process (Melt Pool Size, Temperature, Distortion, Residual Stress, ...)
- Microstructure (Dislocation Density, Grain Size, Precipitate Size, Defects...)
- Properties/Performance (Ultimate Tensile Stress, Fracture Toughness, Creep, Fatigue Crack Growth Rate, Corrosion...)

CM4QC Culture

- Current approaches for Q&C simply do not have procedures for making use of CM results
 - **The naïve expectation - CM predictions may directly replace testing data**
- **Rather, build a culture** in which CM capabilities are used to guide and interpret experiments, development, and testing based on strengths of CM capabilities, while acknowledging their shortcomings
- In the near-term: identify low-risk research activities with a high probability of success for informing Q&C decisions
- **Augment rather than replace existing Q&C practices**, including:
 - Increasing confidence that **material testing is representative of actual components**
 - Reducing the total amount of experimental testing while still **building the necessary confidence** in the results
 - **Improving relevance to real components** with same amount of testing
 - **Reducing variability** to improve designs with same amount of testing

Section 11: Next Steps for Computational Materials-informed Q&C approaches (CM⁴QC Phase II)



Elements of the CM⁴QC Steering Group's Phase II Plan:

- Development of a demonstration exercise (what is possible today, what are the biggest and most important capability gaps).
- IMQCAM STRI
- Socialization and outreach to
 - The aviation industry and corresponding certification authorities
 - Funding agencies and government research laboratories
 - Academia
 - Relevant consortia, professional societies & standards organizations
 - Non-profit organizations
- Off-ramps
- Development of best practice guides

The Foundation of CM⁴QC Validation: NIST-AM Bench



Proceedings of a Workshop



Image: NIST

What is AM-Bench?

A continuing series of highly controlled benchmark measurements for additive manufacturing, with modeling challenge problems, and a corresponding conference series

Primary Goal

To allow modelers to test their simulations against rigorous, highly controlled additive manufacturing benchmark test data

Mechanistic models

Reduced order and surrogate models

Interfaces between models

Consider the Complexities of “real” parts

AM
BENCH 2018

AM
BENCH 2022

AM
BENCH 2025

AM
BENCH 2028



Need, Goal, Digital Twin

- STRI arises from the expense involved in qualifying **safety-critical** 3D printed parts, especially for flight-critical hardware. Motivates physically-based **feedstock-processing-microstructure/defect structure-response workflows that predict performance and fatigue life** based on inputs.
- Central goal of STRI = model-centric workflow that closes the critical gaps between current capabilities and what is necessary for efficient qualification and certification (Q&C) of parts by metals additive manufacturing (MAM), meeting NASA standards.
- The STRI will build and implement a probabilistic [†]Digital Twin (DT) of the MAM physical asset (actual tasks) as a certifiable surrogate for a model-based Q&C process.
- *Our Digital Twin[†] Vision:* will virtually represent the entire **feedstock-processing-microstructure/defect structure-response to life workflow**. Emphasis on end-to-end model system that is responsive to design needs, qualification needs, certification. Less emphasis on numerical avatars (TRL level = 1-3). Reinforced by industry testing and feedback.
- **How will we know that we succeeded?** NASA-MSFC+LaRC (& other Centers) use our modeling toolset + industry uses modeling toolset ... to build trust & increase confidence in metals-AM with higher speed and lower cost.

*STMD – NASA Space Technology Mission Directorate

[†]IMQCAM - Institute for Model-based Qualification and Certification of Additive Manufacturing

ASME VV/UQ 50 Charter: To provide procedures for **verification, validation, and uncertainty quantification** in modeling and computational simulation for advanced manufacturing.

Show value of components of Computational Materials-informed Q&C before capability is fully mature

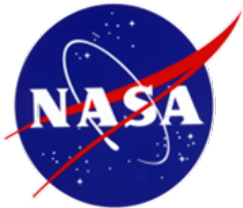
- Demonstrating modeling capabilities (modeling of thermal history, microstructure, defects) in support of establishing similitude (or the lack of thereof...) between the lab test coupon and full-scale parts
- Modeling of residual stresses in AM parts, and utilization of this information in D&DT* assessment; as well as to address potential producibility issues.
- More efficient development of *material allowables* supported by Computational Materials
 - Phase 1 – Informing optimization of test matrices in multi-variate process parameter space.
 - Phase 2 (longer-term) – partial substitution of test data with modeling results.
- “Demonstrator” projects in support of using CM⁴QC for Delta Qual
- Use of CM⁴QC in support of Part Families definition.
- Modeling “effect of defects”, or location-specific critical flaw size assessment to guide NDE and design considerations.
- Acceleration of maturation of new materials? Supporting maturation through the mid-TRL “valley of death”?

Summary



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- Computational Materials Landscape
- Some Regulatory Constraints & Opportunities from FAA
- CM4QC Steering Group, Goals, Membership and Operation
- Highlights of the CM4QC Roadmap
- Elements of the CM4QC Steering Group's Phase II Plan

**Questions or comments:
Please contact us at...**



Ed Glaessgen
e.h.glaessgen@nasa.gov



Michael Gorelik
Michael.Gorelik@faa.gov

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CM4QC Website

[https://www.nist.gov/
programs-projects/cm4qc](https://www.nist.gov/programs-projects/cm4qc)

