

Computational Materials for Qualification and Certification of Process-Intensive Metallic Materials (CM4QC)

An Industry – Government – Academia Steering Group

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Part II - Presented by

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Outline



- Steering Group Goals, Membership and Operation
- Highlights of the CM4QC Roadmap
 - Key Drivers for Increasing the Use of Computational Materials (CM) in the Qualification & Certification (Q&C) Domain for Additive Manufacturing (AM)
 - Key Objectives for Roadmap
 - Industry's Vision and Regulatory Considerations
 - Key Computational Materials Capabilities and Enabling Technologies
 - Validation Metrics, Maturity Assessment Framework and Gaps
 - Approach for Capability Development
 - The CM4QC Ecosystem
- Next Steps

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 **collaboration**.

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

Steering Group Membership



Industry

The Boeing Company*

Lockheed-Martin* / Sikorsky

Raytheon / Pratt & Whitney

General Electric Aviation

Spirit Aerosystems

Honeywell Aerospace

Howmet Aerospace

Southwest Research Institute

Northrup-Grumman Corporation

Textron Aviation

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

Academia

University of Texas at San Antonio*

Carnegie Mellon University*

Vanderbilt University

Pennsylvania State University

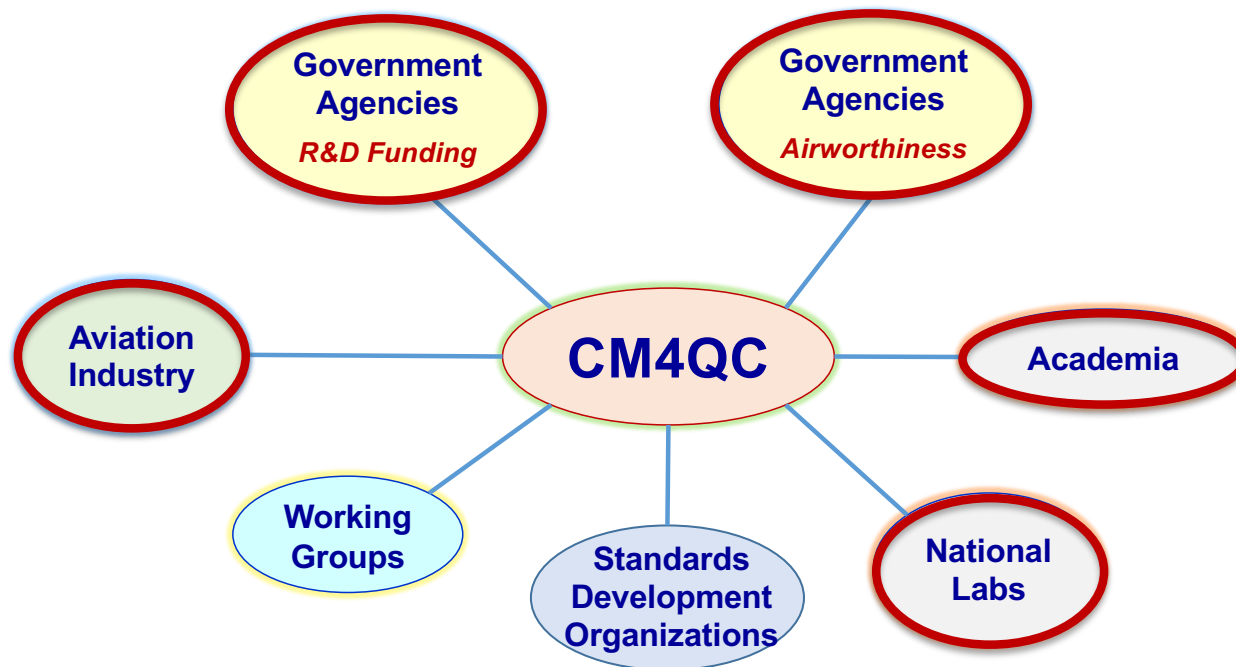
Northwestern University

*CM4QC Leadership Team

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)
- Working Group 3: Development of required **computational materials and measurement capabilities** (Low TRL)



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



Highlights from the CM4QC Roadmap



Maturation of computational materials approaches in qualification and certification for metal additive manufacturing (as an example of process-intensive materials) in aviation

Produced by the Computational Materials for Qualification and Certification (CM4QC) Steering Group

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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Key Drivers for Increasing the Use of CM for Q&C of AM



Business drivers

From Section 1

- Decreased time and cost of Q&C of AM components and systems
- Expanded design space for a given application offered for AM
- Expanded range of applications
- Introduction of economies of scope, beyond existing economies of scale
- Expanded use of AM for producing critical components
- Enhanced design-build-test loop with reduced testing

Technology drivers

- Advances, demonstrated successes, and increased use/acceptance of CM
- Development of digital twins, data standards and digital enterprise
- Advances in high performance computing, artificial intelligence and machine learning
- Advances in V&V methodologies, and maturation of credibility assurance frameworks
- Advances in sensitivity and uncertainty quantification methods
- Increases in the availability of high-quality validation data
- Improvements and increased availability of in-situ and ex-situ measurement systems
- Advances in relevant technical standards and industry best practices

Key Objectives for this Roadmap

Development of a pathway towards Computational Materials-informed Q&C

From Section 2

Detailed Objectives include

- Document industry vision of the future state for the use of CM
- Identify key considerations and enablers required to increase airworthiness and certifying authorities' acceptance of computational methods
- Identify current gaps and key enabling CM capabilities
- Identify R&D investment opportunities
- Develop a framework to evaluate the maturity level of CM simulations
- Initiate a paradigm shift in the aerospace industry's use of CM tools
- Assess the state-of-practice of CM for potential application in Q&C
- Increase dialogue among the stakeholder organizations
- Encourage development of relevant guidance/standards
- Inform academia about training and education gaps

Industry's Vision for AM

- Print *worthy* components anywhere and anytime. Worthiness is dependent on the situational requirements and can refer to airworthiness, cost, or other attributes.
- Expand manufacturing possibilities and emphasizing “economies of scope” operational models
- Reduced lead-time for manufacturing new, complex components
- Reducing the cost for small volume or even single-part production
- Reduced part weights, subassembly part counts, and inventories

From Section 3

Key business benefits of Computational Materials-informed Q&C

- Reduced time and resources for Q&C of high-consequence aviation components
- Improved part performance through design flexibility
- Accelerated development of tailored alloys for targeted AM applications
- Development and acceptance of new AM machine architectures
- Accelerated “delta qualification” of machines with minor hardware/software changes
- Quantified and mitigated build variations
- Implementation of smarter testing inclusive of the variation across the part
- Use of AM build process and performance modeling to focus limited NDE resources
- Promotion of performance-risk-based decisions using computational materials engineering, including comprehensive UQ assessment

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

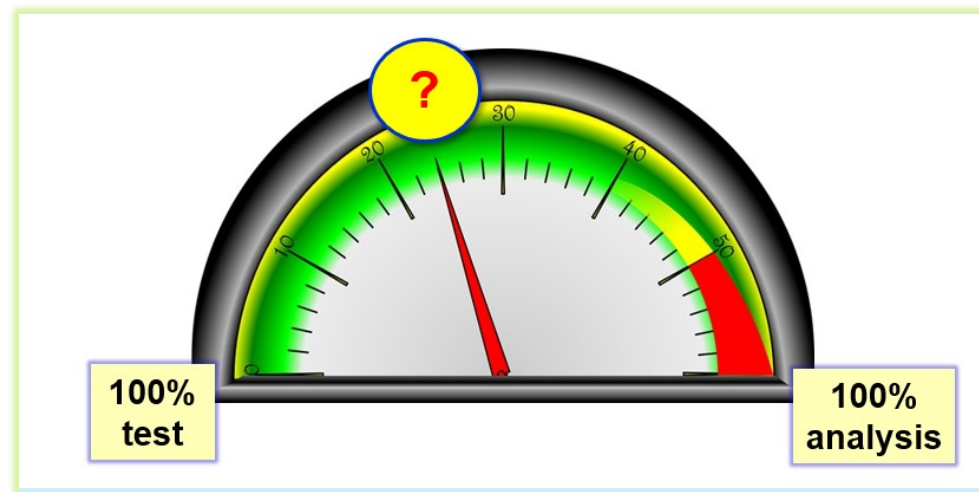


From Section 4

Key drivers

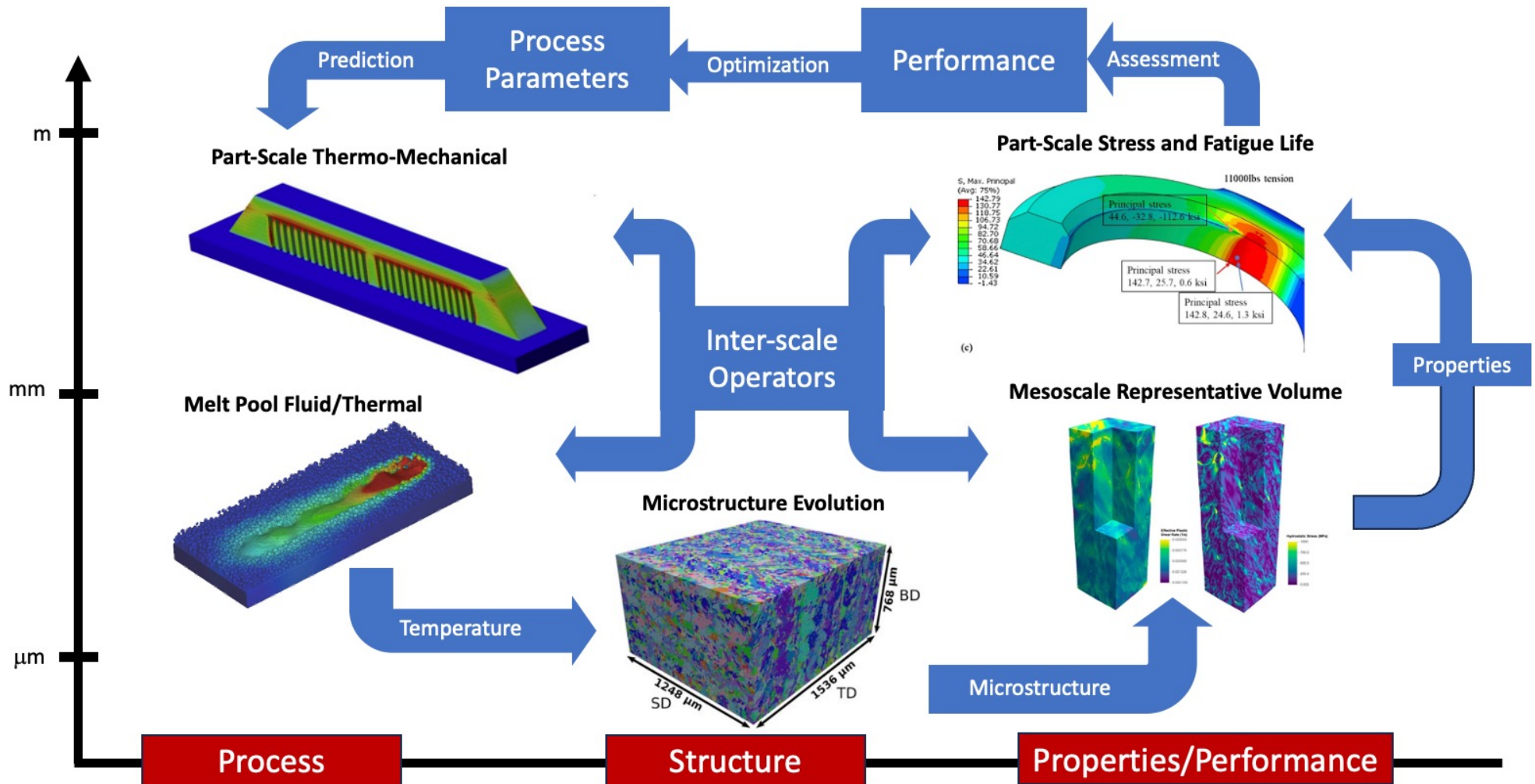
- Gradual **reduction** in conventional **Q&C test matrices**
- Optimization of material test matrices informed by CM insights (i.e., **obtaining the most valuable information from testing**)
- Exploring the corners and fringes of the multi-dimensional process parameters space to **fully capture material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

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



Key Computational Materials Capabilities & Enabling Technologies

From Section 5



PSP/P Modeling Framework

“State of Practice” Assessment of Computational Materials Capabilities



From Section 6

Includes Brief Assessments of:

Process

- Simulation of Powder Flow
- Computational Thermodynamics
- Macroscopic Heat Flow Simulation
- Residual Stress Prediction
- Heat Flow at the Individual Track Level
- Fluid Flow in Melt Pool Simulations

Structure

- Microstructure Simulation

Property/Performance

- Property & Performance Prediction

Key Cross-Cutting Topics

- Computing Capacity
- Data Storage
- Material Properties & Constitutive Models
- V&V and UQ

Validation Metrics

From Section 7

- 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.

CM Maturity Assessment Framework*



From Section 8

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 are 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.

Gaps Limiting Maturation and Adoption of Computational Materials in the Q&C Domain (1 of 2)



From Section 9

- Prediction of
 - **Process-microstructure relationships** (e.g., phases, precipitates, and grain size)
 - **Microstructure-property relationships** (e.g., mechanical and physical properties, various functional properties)
 - **Property-performance relationships** (e.g., strength, fatigue life, damage tolerance, durability, and reliability), including critical aspects such as surface finish (including surface particles), defects, complex loading histories, and environmental and temperature conditions
 - **Residual stress and distortion**
- Build reproducibility
- **NDE**, including for process development, process qualification, manufacturing, and in-service performance
- Quantitative assessment of **performance uncertainty and reliability**

Gaps Limiting Maturation and Adoption of Computational Materials in the Q&C Domain (2 of 2)



From Section 9

- Acceptance by industry and regulatory agencies
 - Incremental with rigorous validation testing
 - Requires trust in models and clear business cases
- Improvements to ease-of-use of software
 - Software must be easy to use and run on laptops or workstations
 - Non-proprietary input/output formats
 - Publicly available validation data such as provided by AM Bench
- Availability of material property data
- Integration of Uncertainty Quantification
- Resources to conduct side-by-side CM-related and conventional Q&C activities, until CM tools are widely accepted as being viable
- Improvements in transitioning non-commercial AM codes to commercial platforms with version control, continued maintenance, linkages, etc.
- Educational improvements leading to increased availability of a CM-informed work force

A Phased Approach for Development of a Capability for Computational Materials-informed Q&C



From Section 10

Near-term (1-5 years)

- Identification of approaches that incorporate **existing commercial software including guiding conventional Q&C activities**, e.g., designing experiments or guiding testing practices

Mid-term (5-10 years)

- Development of **partnerships** between aerospace organizations, software vendors, national laboratories, and universities targeting emerging techniques for CM and accelerating their incorporation into commercial tools and Q&C practices
- Includes support from manufacturers and regulators to **identify the most critical areas of research**

Long-term (>10 years)

- Development of **new CM techniques that dramatically expand the capabilities of computational simulations and their application to Q&C**
 - Expand the physical fidelity and accuracy of models
 - Focus on methods that dramatically reduce computational expense
 - Exploit highly efficient computing paradigms (e.g., GPUs)

How Can Computational Materials Augment (Rather than Replace) Existing Q&C practices?

- Investment in Computational Materials capability development
- Transition to next-generation AM machines to enable Computational Materials-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 Computational Materials results
 - The naïve expectation is that 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

Next Steps

Publication of **this document is just the first step** in a process that includes:

- A **public rollout** through presentations at dedicated annual symposia
- **Continued public engagement** through workshops and symposia
- **Socialization** of new Computational Materials-informed Q&C approaches throughout the aviation industry and corresponding certification authorities
- Development of **best practice guides**
- **Outreach** to
 - Funding agencies
 - Government research laboratories
 - Academia
 - Relevant consortia, professional societies, and standards organizations
- Extension **beyond Additive Manufacturing** (to other PIM technologies)

Summary



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Questions: Please contact us at...



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