

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

An Industry – Government – Academia Steering Group

CM4QC Annual Workshop

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Approved for Public Release



Around the room...

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

Workshop Goal, Format & Importance of Reviewer Input



The ***primary goal*** of this ***workshop*** is to:

- **Answer questions about the CM4QC Roadmap** that will help the Red and Orange Teams to more effectively review the document

The ***format*** of this ***workshop*** is:

- A **section-by-section** discussion
- **Very brief summaries** from the authors **followed by an interactive discussion** with the reviewers

The importance of reviewer input

- CM4QC has developed this document / contents during the past 4 years
- The work of over two dozen authors and additional contributors
- We need a fresh perspective
 - **What did we miss? What did we get wrong? What is extraneous?**
 - What questions do you have for us?

Roadmap Outline



Section	Focus
1	Background
2	Scope
3	Industry's Vision
4	Regulatory Considerations for CM Acceptance
5	Key Computational Materials Capabilities & Enabling Technologies
6	"State of Practice" Assessment of Computational Materials Capabilities
7	Key Elements & Associated Methods for Computational Materials Verification, Validation & Uncertainty Quantification
8	Computational Materials Simulation Maturity Level Assessment Framework
9	Technology Maturation Path
10	R&D investment opportunities for CM tools
11	CM Ecosystem Maturation Path
12	Next Steps

Section 1: Background



The purpose of this section is to **introduce the need for a technologically-updated paradigm for Qualification and Certification of Process Intensive materials**. Current focus is on additively manufactured metallic materials.

- Development of a Computational Materials-informed paradigm offers the promise of decreasing the time and cost of Q&C and is enabling to certain aggressive paradigms* (e.g., effective use of graded material compositions, in-space manufacturing)
- Requires a significant shift of both the engineering paradigm and the industry/regulatory culture
- Primary barriers to realizing these benefits are maturation / validation of required modeling / measurement capabilities and acceptance (trust) by both industry and regulators

* Beyond the scope of this roadmap

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

Section 2: Scope

The purpose of this section is to:

- Identify the **objectives and desired impacts** of the roadmap
- Highlight the **overarching gaps** limiting maturation of Computational Materials in the Q&C domain
 - **Lack of acceptance** by regulatory agencies and industry
 - **Insufficient maturity** of CM and associated capabilities for use in Q&C
 - **Inadequate metrics** for assessing the maturity of CM for use in Q&C
 - Lack of publicly available **validation measurement data**
 - **Limited capabilities for UQ** of CM simulations
 - **Insufficiently prepared workforce**
- Provide an overview of the **structure of the roadmap**
 - **Introductory material** (Sections 1 through 4)
 - **Current state** of CM for AM Q&C (Sections 5 through 7)
 - **Assessing and maturing** CM capabilities for Q&C (Sections 8 and 9)
 - **Investment opportunities** (Sections 10 and 11)

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

Workshop Agenda (1 of 2)



0930-1630 Section-by-Section Discussion of Roadmap

Format: Brief (5 min) summary followed by interactive discussion

Time	Topic	Facilitator	Scribe
0930-1000	Section 3: Industry Vision	D. Lamm	J. Pribe & L. Das
1000-1015	Break		
1015-1045	Section 4: Regulatory Considerations	M. Gorelik	A. Kitahara & S. Yeratapally
1045-1115	Section 5: Key Capabilities and Technologies	V. Venkatesh & A. Rollett	S. Hocker & L. Das
1115-1145	Section 6: State of Practice Assessment	A. Rollett	S. Hocker & L. Das
1145-1200	Open Discussion		
1200-1300	Lunch		

Workshop Agenda (2 of 2)



Time	Topic	Facilitator	Scribe
1300-1330	Section 7: V&V/UQ	S. Mahadevan & H. Millwater	J. Pribe & S. Hocker
1330-1400	Section 8: Simulation Maturity Level Assessment	E. Schwalbach & L. Levine	A. Kitahara & G. Weber
1400-1445	Section 9: Technology Maturation Path	C. Battaile & L. Levine	G. Weber & S. Yeratapally
1445-1500	Break		
1500-1545	Section 10: R&D Investment Opportunities for CM	E. Glaessgen & A. Plotkowski	G. Weber & A. Kitahara
1545-1630	Section 11: CM Ecosystem Maturation Path	M. Gorelik & A. Plotkowski	S. Yeratapally & J. Pribe
1630-1655	Path Forward	D. Lamm, A. Peralta & E. Glaessgen	
1655-1700	Closing Comments	M. Gorelik & E. Glaessgen	

Discussion of Sections 3 – 11 of 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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Section 4: Regulatory Considerations



The purpose of this section is to provide a high-level overview of regulatory considerations and potential future actions in the context of Computational Materials-informed Q&C

- Current state of Q&C, entry points and regulatory enablers
- Key drivers for use of Computational Materials in the Q&C domain
- Converged future state: balance between testing and Computational Materials
- Future work needed to achieve regulatory acceptance

Regulatory Considerations for Acceptance of Computational Materials-informed Q&C (1 of 2)

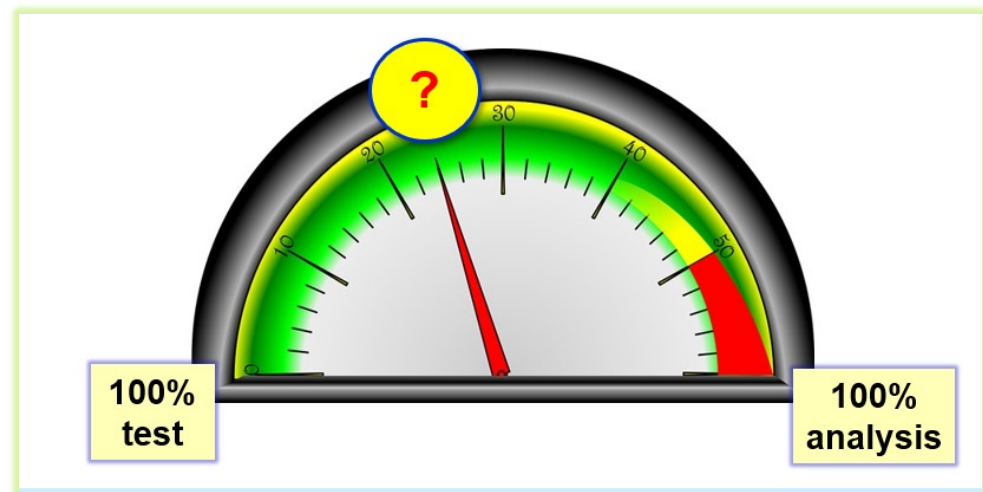


From Section 4

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***



Regulatory Considerations for Acceptance of Computational Materials-informed Q&C (2 of 2)



From Section 4

Future Work

- Identification of regulatory gaps impeding broader use of CM and development of a plan to address these gaps
 - Development of regulatory guidelines and/or industry standards for acceptable levels of Verification, Validation and Uncertainty Quantification (VVUQ) for CM, commensurate with the application's criticality, simulation maturity level and extent of CM utilization
 - Development of methodologies and guidelines for generation of “hybrid” allowables where conventional test data is supplemented by CM model predictions
 - Development of Credibility Assurance Framework (CAF) considerations from ASME VVUQ-90 for use of CM models, especially in high-criticality applications
 - Development of illustrative examples that can be used for training and education of regulators and applicants
- Requires close collaboration between regulators and industry

Section 10: R&D Investment Opportunities for CM Tools (1 of 2)



- The purpose of this section is to describe the major classes of CM capabilities and **where R&D investment is needed**
- Broken down into key **categories**:
 - Physics – process
 - Physics – microstructure
 - Physics – properties and performance
 - Software – infrastructure
 - Software – accelerated computation
- Table 10.1 summarizes an estimate of the **status of a variety of capabilities**, and the level of difficulty involved with further improvement

Table 10.1

Thematic Area	Topic	Status		Difficulty	
		✗ Ideation	✗ Highly challenging	✗ Development	✗ Difficult
		⚠	⚠	⚠	⚠
		✓ Ready	✓ Easy	✓	✓
Physics – Process	1. LOF porosity [51]	⚠	✓	⚠	✓
	2. Residual stress [87]	✓	✓	⚠	⚠
	3. Distortion [87]	⚠	✓	⚠	⚠
	4. Full part thermal history [167,168]	⚠	✓	⚠	⚠
	5. Chamber scale effects (build thermal history/gas flow etc.)	⚠	✓	⚠	⚠
	6. Keyhole and entrapped gas porosity [169]	⚠	✓	✗	✗
	7. Spatter prediction and induced defects	✗	✗	✗	✗
	8. Melt pool dynamics (e.g., fluid flow, keyholing) [170,171]	⚠	✓	✗	✗
	9. Solidification conditions [170]	⚠	✓	✗	✗
	10. Melt pool variability	✗	✗	✗	✗
	11. Gas flow, plume, and laser interactions [172]	✗	✗	✗	✗
	12. Powder flow and effects [173]	✓	✓	⚠	⚠
	13. Powder recycling	✗	✗	✗	✗
	14. Dissolved gas porosity [174]	⚠	✓	✗	✗
	15. Surface roughness	✗	✗	✗	✗
Physics – Microstructure	16. Computational Thermodynamics [175]	✓	✓	✓	✓
	17. Thermo-kinetics	✓	✓	⚠	⚠
	18. Grain scale microstructure [63,176,177]	⚠	✓	✗	✗
	19. Sub-grain microstructure [178,179]	⚠	✓	⚠	⚠
	20. Dislocation structure	✗	✗	✗	✗
	21. In-process cracking [180]	⚠	✓	✗	✗
Physics – Properties and Performance	22. Static mech. properties (YS, work hardening) [181]	⚠	✓	⚠	⚠
	23. Static mech. Properties (Ductility, UTS)	✗	✗	✗	✗
	24. Creep	✗	✗	✗	✗
	25. Fatigue [182,183]	✗	✗	✗	✗
	26. Toughness	✗	✗	✗	✗
	27. Environmental effects	✗	✗	✗	✗
	28. Part scale geometric effects [184]	✗	✗	✗	✗
Software Infrastructure	29. Non-intrusive UQ [162,163]	✓	✓	⚠	⚠
	30. Intrusive UQ	✗	✗	✗	✗
	31. Model validation	✓	✓	⚠	⚠
	32. Model coupling infrastructure	✓	✓	⚠	⚠
Software – Accelerated Computation	33. Machine learning/surrogate models [185]	⚠	✓	⚠	⚠
	34. Physics-based reduced-order models	⚠	✓	✗	✗
	35. Hybrid ML/Physics models	✗	✗	✗	✗

Section 10: R&D Investment Opportunities for CM Tools (2 of 2)



- Investment opportunities are characterized by timeframe and the level of challenge for maturation
- The purpose is to inform stakeholders regarding needs that may align with their mission space
- Discusses near, mid, and long-term timelines and possible investment strategies
- Table 10.2 provides a number of opportunities (i.e., challenges vs. industry need)

Table 10.2

Challenge → Industry Need ↓	Straightforward to Implement and/or available in commercial codes	Moderately Challenging and/or moderate resources required	Challenging to Develop and/or Requires Major Computing Resources
Immediate Benefit/Need	- Full field, full part thermal history via simplified heat flow models (e.g., lumped layer) - Defect prediction: LoF porosity - Residual elastic strain - CALPHAD: equilibrium phase diagrams - Thermokinetics: kinetics of precipitation e.g., time-temperature transformation (TTT) or continuous cooling transformation (CCT) curves for homogeneous composition	- Scan path resolved full field, full part thermal history (heat flow only) via ML or reduced order models - Structure-Properties: YS - Defect prediction: keyhole porosity via ML - Distortion from thermal contraction - CALPHAD Scheil calculations for solidification - Thermokinetics: kinetics of precipitation (TTT, CCT) [where diffusion data is not available, or for highly heterogeneous composition] - Thermokinetics with transport (for TTT/CCT) via an empirical model based on a calibrated physics model.	- Melt pool resolved full field, full part thermal history via full-field thermal flow - Defect prediction: keyhole porosity via full-field fluid flow simulation
Strong Benefit/Need	- Defect prediction: spatter generation via ML - Gas flow in the chamber [commercial] - Melt pool variability (for LoF prediction, e.g.) via ML [data hungry]	- Processing-Structure: Micro-segregation prediction for homogenization schedules - Melt pool variability (for LoF prediction, e.g.) via simulation - Melt pool variability via an empirical model based on a calibrated physics model.	- Structure-Properties: fatigue, creep, and corrosion - Fluid flow (full physics) in the melt pool [commercial]
Clear Benefit in the long term	Physics informed AI/ML methods that combine simulation and process data	- Melt pool temperature, fluid flow & vaporization - Process-structure: grain-scale microstructure for texture, grain shape, via ML [data hungry]	- Processing-Structure: grain-scale microstructure for texture, grain shape via full-field simulation (CA, KMC) - Structure-properties: Development of dislocation structures

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)

Section 11: CM Ecosystem Maturation Path



The purpose of this section is to describe the main components of the CM ecosystem

- Investment in CM capability development (Section 10)
- Transition to next-generation AM machines to enable Computational Materials-informed Q&C
 - Machine architectures that support data collection and model definitions consistent with QC practices
- Characterization and data practices for calibration, validation, and machine learning
- CM4QC culture
 - Building an engineering culture that accepts CM capabilities
- Development of CM-appropriate regulatory standards
- CM Education and workforce development
 - Define some educational goals for undergraduate and graduate students, and for continuing education of current engineers

Characterization and Data Practices for Calibration, Validation, and Machine Learning



From Section 11

- Need **pedigreed data** for model inputs, model validation, and for ML training
- Wide range of relevant techniques, ranging from common to highly specialized
- Tables 11.1 (right) and 11.2 (not shown) seek to define the **availability of measurement techniques** and their degree of uncertainty for relevant inputs and outputs, respectively

Table 11.1

Thematic Area	Data	Characterization Techniques	Current status	Degree of Uncertainty
			✓ Lab scale ⚠ Limited/challenging ✗ Rare/highly challenging	✓ Low ⚠ Med ✗ High
Physics – Material properties	Density	Archimedes, pycnometry	✓	✓
	Coefficient of thermal expansion (T)	Dilatometry	✓	✓
	Specific heat/latent heat (T)	Differential scanning calorimetry (DSC)	✓	✓
	Thermal diffusivity	Laser flash	✓	✓
	Freezing range	DSC	✓	⚠
	Boiling temperature	DSC	⚠	✓
	Vapor Pressure	Heat pipe	✓	✓
	Surface tension (T)	Levitation droplets	✗	✗
	Viscosity	Rheometer, levitation droplets	✗	⚠
	Fresnel absorption	Calorimetry	✗	✗
Physics – Process	Scan path	Machine vendor	✗	✗
	Layer height	Machine vendor	✓	✓
	Laser power	Machine vendor and calibration	✓	⚠
	Laser power distribution function	Imaging	⚠	✗
	Gas flow	Anemometer, Schlieren	✗	⚠
	Gas composition	Oxygen sensors, humidity sensors, etc.	✓	✓
	Ambient temperature	Weather channel	✓	✓
	Build plate temperature	Thermocouple	✓	⚠
	Powder size	Laser diffraction, microscopy, X-ray CT, sieve	✓	✓
	Powder composition	Inductively coupled plasma	✓	✓
Physics – Microstructure				
	Diffusion coefficients	Diffusion couples, isotope tracers	✓	✓
	Thermo-kinetic data			
	Liquid diffusion coefficients	molecular dynamics (MD)	✗	✗
	Solid/liquid surface energy	Wolff crystals, MD	✗	✗
	Solid/solid surface energy	Density functional theory (DFT)	⚠	⚠
	Nucleation density liquid to solid	EBSO	✗	✗
	Nucleation density solid-solid	Precipitate characterization (e.g., TEM)	✗	✗
	Nucleation undercooling (distribution)		⚠	✗
Physics – Properties	Liquidus surfaces		✓	✓
	Partition coefficients (T)		✓	⚠
	Dislocation density	Diffraction, microscopy	⚠	⚠
	Grain size and texture	Microscopy (EBSD)	✓	✓
	Precipitate size and fraction	Microscopy (SEM, TEM, atom probe tomography (APT))	✓	✓
	Phase identification	Diffraction,	⚠	⚠

- 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 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
 - **How to phase the use of CM in a manner that builds trust**
- 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**)