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Computational Materials for Qualification and Certification (CM4QC) Strategy Document:
Maturation of Computational Materials Methods for Aviation-Focused Qualification and Certification of Metal Additive Manufacturing (as an Example of Process-Intensive Materials)

March 2026

Prepared for

Department of Transportation
Federal Aviation Administration
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March 2026

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Preface

Computational Materials for Qualification and Certification (CM4QC) began as a conversation between Ed Glaessgen and Michael Gorelik in Ed's office at NASA Langley Research Center (LaRC) in the Fall of 2019. The resulting concept, "maturing Computational Materials as a future component of industry's approach for Qualification and Certification of Additively Manufactured (AM) metallic materials," led to a workshop at LaRC in January 2020 that begot the CM4QC steering group who, collaboratively, developed this document.

The CM4QC steering group is divided organizationally by Technology Readiness Level (TRL) into three working groups (WGs) led by co-chairs as:

- WG 1: high-TRL, focused on assessing industry and regulatory requirements and determining how Computational Materials can reduce risk, time and cost of new product development, insertion of new materials and acceptance of new processes, while meeting the uncompromising regulations associated with safety-of-flight;
- WG 2: mid-TRL, focused on bridging the "Valley-of-Death" from academic/research methods to validated engineering capabilities;
- WG 3: low-TRL, focused on assessing the suitability of current Computational Materials-related capabilities, many of which are currently employed under the banner of Integrated Computational Materials Engineering (ICME), and identifying lower TRL research, mostly-academic, capabilities that are candidates for further maturation across the mid-TRL Valley of Death. Recognizing the differences between V&V requirements that enable computational materials methods to be used in ICME paradigms and the substantially higher V&V requirements that will enable computational materials methods to be trusted by regulators, is at the core of CM4QC.

The co-chairs are domain experts and technical leaders who skillfully led each of their working groups to develop the impactful content within this document. Additionally, two CM4QC members, Lyle Levine and Eddie Schwalbach, took on the formidable tasks of compiling input from the working groups and making many of the initial edits to the document that you are about to read. The external Review Teams, consisting of a formal Red Team composed of seven notable SMEs representing aerospace Q&C, computational materials, and metal AM and an informal Orange Team, composed of talented colleagues of the steering group members, provided thorough and insightful critique of the original draft of the document.

Together with the Review Teams, CM4QC is a unique volunteer organization that, while bringing distinct and invaluable technical viewpoints from industry, government and academia, is united by a common focus. This framework combined with a highly experienced and dedicated membership makes the CM4QC steering group more than the sum of its parts. Even beyond the domains of Computational Materials, Q&C and AM, CM4QC can be viewed as a collaborative model for bringing engineers and scientists together to bridge the technological Valley-of-Death and address the Nation's most difficult technical challenges. Perhaps the most significant outcome from the CM4QC steering group is the steering group, itself.

It has been our privilege to closely work with each member of CM4QC and its Review Teams throughout the process of developing this document. We thank everyone involved for sharing their insight, knowledge and wisdom.

Ed Glaessgen and Michael Gorelik
CM4QC Co-chairs / Co-organizers, February 2026

Computational Materials for Qualification and Certification (CM4QC) Steering Group Membership

<u>Government</u>

Edward H. Glaessgen, National Aeronautics and Space Administration	CM4QC Co-Chair
Michael Gorelik, Federal Aviation Administration	CM4QC Co-Chair
Lyle Levine, National Institute of Standards and Technology	Working Group 2 Co-Chair, Lead Editor
Corbett Battaile, Sandia National Laboratories	Working Group 3 Co-Chair
Michael Kane, U.S. Army, Aviation and Missile Center	
Nam Phan, U.S. Navy, Air Systems Command	
Alexander Plotkowski, Oak Ridge National Laboratory	
Edwin Schwalbach, U.S. Air Force Research Laboratory	Assistant Editor

<u>Industry & Research Institutes</u>

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Markus Heinimann[2], Howmet Aerospace	
Pete Kantzos, Honeywell Aerospace	
Alonso Peralta-Duran, Honeywell Aerospace (retired)	Co-chair at Large
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Deborah Whitis, General Electric Aerospace	

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Anthony Rollett, Carnegie Mellon University	Working Group 3 Co-Chair
Sankaran Mahadevan, Vanderbilt University	
Caglar Oskay, Vanderbilt University	
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<u>Working Group 1:</u> Understanding industry priorities and key regulatory implications (High TRL)
<u>Working Group 2:</u> Strategies for maturing and transitioning research to engineering (Mid TRL)
<u>Working Group 3:</u> Developing required computational and measurement capabilities (Low TRL)

[1] Current affiliation: BAE Systems
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Acknowledgements

This document, *Computational Materials for Qualification and Certification (CM4QC) Strategy Document: Maturation of Computational Materials Approaches for Aviation-Focused Qualification and Certification of Metal Additive Manufacturing (as an Example of Process-Intensive Materials),* is the culmination of over five years of work by subject matter experts from industry, government, and academia as part of the informal CM4QC steering group. CM4QC was assembled to develop a comprehensive strategic framework and maturation path for increasing the use of computational materials approaches in the aviation qualification and certification (Q&C) domain with an initial focus on additive manufacturing (AM).

Virtual meetings of the three Working Groups (WGs) were held every two weeks, leadership team (CM4QC and WG co-chairs) meetings were held weekly, and in-person meetings were held yearly once the end of the COVID-19 pandemic restrictions made this possible. The co-chairs sincerely thank all the CM4QC members for their professionalism, involvement, and dedication to this effort. We also thank both the Orange Team Reviewers and the Red Team Reviewers for sharing their expertise and insight during the CM4QC Roadmap Review process. Finally, we thank the various government, industry, and academic organizations that supported the CM4QC members and reviewers throughout this process.

The informal Orange Team Reviewer membership included the following experts:

Suresh Babu, University of Maryland
Thomas Broderick, FAA
Scott Cochran, Lockheed Martin
Erik Frankforter, NASA LaRC
Brian Gockel, Lockheed Martin
Markus Heinimann, ATI
Nik Hrabe, NIST
Kevin Jurrens, NIST
Orion Kafka, NIST
Andrew Kitahara, Analytical Mechanics Associates
Bruce Kramer, NSF
Brandon Lane, NIST
Mick Maher, Maher-Associates
Steve Mates, NIST
Joshua Pribe, Analytical Mechanics Associates
Brandon Ribic, America Makes
Brodan Richter, NASA LaRC
Richard Russell, Barnes Global Advisors
Michael D. Sangid, Purdue University
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Albert To, University of Pittsburgh
Mark VanLandingham, NIST
George Weber, NASA LaRC
Bryan Webler, Carnegie Mellon University
Saikumar Yeratapally, Science and Technology Corporation

The formal Red Team Reviewer membership included the following experts:

Charles Babish	United States Air Force
Dale Ball	Lockheed Martin
Brad Cowles	Cowles Consulting, LLC
David Furrer	Pratt & Whitney
Somnath Ghosh	Johns Hopkins University
Ben Thacker	Southwest Research Institute
Douglas Wells	NASA Marshall Space Flight Center

The Red Team and all but one of the Orange Team members were not involved in the development of this document and are not CM4QC steering group members, thus representing *independent* viewpoints and expertise.

All the reviewer comments and suggested changes were either directly incorporated into the revised document; or, at a minimum, discussed and dispositioned by the CM4QC members. A careful record of how each individual comment was addressed has been kept by the document's editors. Some of the suggested changes that were not incorporated will be considered as guidance for follow-on CM4QC documents.

Contents

Why was this report written?

This report was written to address the U.S. aviation industry's need to increase the efficiency of qualification and certification (Q&C) of process-intensive aviation components through the maturation and adoption of computational materials (CM) methods. A key challenge in the introduction of these CM approaches is overcoming the *valley of death*, where promising low-TRL CM-based Q&C technologies struggle to progress toward industry deployment. Despite the inherent promise of CM capabilities, their application has been primarily limited to the early phases of the product development cycle due to insufficient trust in CM outputs, fragmented industry adoption, regulatory acceptance, and a lack of standardized frameworks for integrating computational methods into established Q&C practices.

As the pace of technological advancement accelerates globally, increasing the speed and reducing the cost of innovation are critical to ensuring that U.S. industry remains competitive and can rapidly adopt new materials and manufacturing processes. By outlining industry needs, regulatory considerations, key software capabilities, validation strategies, uncertainty quantification, and the current state of computational methods and practices, this report provides a roadmap for building confidence in CM tools and integrating them into Q&C frameworks. It also introduces a simulation maturity framework and maturation pathways within a broader CM ecosystem, concluding with recommended next steps to drive progress in this critical domain.

Document Structure

The primary subject matter of this document is laid out in five consecutive parts as shown below. These are followed by concluding remarks and eight appendices that include additional details, and an example related success story for the application of CM to residual stress modeling. Acronyms are defined separately in the preface material, the Executive Summary, and the main document. They are not redefined in each section but are listed in Appendix VIII.

A. Introductory material (Sections 1 and 2):

Section 1 sets the stage by providing a background and context, a clear problem statement, a bulleted list of business and technological drivers, and a brief description of several past and existing government initiatives and efforts in this technology space. Section 2 then describes the scope of the document with an emphasis on objectives, expected impacts, and gaps.

B. Industry's vision and regulatory considerations (Sections 3 and 4):

Section 3 lays out the drivers for CM from an industry perspective with a clear description of the current and desired future state of AM qualification. Section 4 presents complementary considerations from the regulatory perspective that must be addressed before CM approaches can be accepted as a part of the Q&C process.

B. Current state of CM for AM Q&C (Sections 5 and 6):

Section 5 introduces the current state of CM for AM Q&C by briefly describing the key CM tools used for simulating AM process-structure-property-performance (PSPP) behaviors and relationships along with the corresponding supporting technology needs. Section 6 rounds out the discussion of the current state by summarizing the state-of-the art for verification and validation (V&V) and uncertainty quantification (UQ).

C. Assessing and maturing CM capabilities for Q&C (Sections 7 and 8):

Any process for bringing CM engineering approaches into the Q&C domain requires a methodology for assessing the various factors that impact the maturity of a CM simulation for a given application. Section 7 presents such a framework that is based upon earlier work on assessing integrated computational materials engineering (ICME) approaches. Section 8 discusses broad needs for maturation based upon technological and engineering drivers with some examples showing how fundamental research can impact engineering requisites.

D. Investment opportunities (Sections 9 and 10):

Section 9 and Section 10 complete the narrative by providing a detailed look at the current state of CM tools and the CM ecosystem with an emphasis on investment opportunities.

Who should read this report and how should they approach it?

CM approaches have the potential to significantly decrease the time and cost of Q&C practices and realize the potential of AM in the aviation industry. Ultimately, these benefits can be extended to other industrial sectors and process-intensive material technologies making this maturation plan pertinent to a wide range of stakeholders having different interests and needs. The key stakeholders for this report are given below. While the authors recommend reading the entire document, it is recognized that individuals have time constraints so we provide suggestions for which sections may be most useful. This reading guide is intended to inform each group about CM capabilities that they may benefit from using, especially for developing Q&C packages. Therefore, this section is primarily informational, albeit with the goal of setting a path toward gradual acceptance of CM within the Q&C domain. All readers are recommended to read Section 7 to understand the high level of V&V rigor that will be required before CM can be trusted within the Q&C domain.

Regulatory Officials and Technical Warrant Holders who are chiefly responsible for the Q&C of AM parts can read the document to gain a sense of what to expect in a Q&C package that uses the results of CM as part of the evidence file by, e.g., amplifying or filling in gaps in experimental results.

A suggested reading path is as follows:

Section 3 Industry's Vision
Section 4 Regulatory Considerations for CM Acceptance
Section 5 Key Computational Materials Capabilities & Enabling Technologies
Section 7 Computational Materials Simulation Maturity Level (SML) Assessment Framework

Chief Engineers and **Managers** who are primarily responsible for reviewing Q&C packages for AM parts and implementing strategic Q&C approaches will gain an understanding of the potential of CM tools to accelerate Q&C. The document is intended to help them understand how Q&C packages for flight hardware can benefit from CM tools to accelerate the Q&C process and manage risk. It is also intended to give a sense of how the CM toolbox has built upon the successes found in ICME [1]. This document may also assist with determining the appropriate allocation of engineering resources for these CM approaches.

A suggested reading path is as follows:

Section 3 Industry's Vision
Section 5 Key Computational Materials Capabilities & Enabling Technologies
Section 7 Computational Materials Simulation Maturity Level (SML) Assessment Framework
Section 9 R&D Investment Opportunities for CM Tools
Section 10 CM Ecosystem Maturation

Design, Mechanical, and System Engineers should find value in this document to understand the CM tools that exercise the capabilities and address the limitations of AM. For example, it offers guidance in terms of Q&C packages along with connections to mechanical properties and design practices. It also helps with understanding the pedigree of design data based on the CM tools. It provides insight into the capabilities and limitations of AM for those who require detailed process awareness to execute their role in the Q&C processes. Introducing AM almost always leads to re-optimization of part design, which implies concurrent design of part, process, and material. Incorporating feedback from CM tools should lead to improved design and manufacturability. Utilization of CM tools enables multi-objective optimization against cost, design/re-design iterations, material usage, performance, etc.

A suggested reading path is as follows:

Section 3 Industry's Vision
Section 4 Regulatory Considerations for CM Acceptance
Section 5 Key Computational Materials Capabilities & Enabling Technologies
Section 6 Key Elements & Associated Methods for Computational Materials Verification, Validation & Uncertainty Quantification
Section 7 Computational Materials Simulation Maturity Level (SML) Assessment Framework

Production/Industrial/Quality Engineers and Technicians in industry (e.g., product development teams) should find guidance for which CM tools are likely to help them do their jobs when confronted with the need to develop Q&C packages for new parts. The CM tools described herein can assist in developing a stable production process that leads to a Qualified Materials Process defined in standards documents (e.g., NASA-STD-6030 [2]). It also provides guidance for identifying what simulation techniques are available to the engineer as software tools for predicting aspects of the printing process that relate to part performance and build reproducibility. The simulation results can then be incorporated into the Q&C evidence file. The engineer must show how they verified correct operation of the code employed (e.g., numerical solution of a standard heat flow problem), and how they validated the code against measurement data. Superior Q&C packages will include UQ for the outputs. In certain circumstances, it may be appropriate to claim credit for design-by-analysis.

A suggested reading path is as follows:

Section 3 Industry's Vision
Section 4 Regulatory Considerations for CM Acceptance
Section 5 Key Computational Materials Capabilities & Enabling Technologies
Section 6 Key Elements & Associated Methods for Computational Materials Verification, Validation & Uncertainty Quantification
Section 7 Computational Materials Simulation Maturity Level (SML) Assessment Framework

Materials and Process Engineers are offered similar guidance as for the previous areas of engineering but with greater emphasis on underlying processes and CM approaches, such as microstructure evolution and computational thermodynamics. Some may be familiar with CM tools and therefore will benefit the most by following the motivations of CM tool usage starting with the industry vision and key regulatory gaps in AM Q&C. Others who may be familiar with Q&C but are perhaps unfamiliar with CM tools may find greater benefit with the suggested reading path described for design, mechanical, and system engineers in a previous paragraph. Responsibility for materials selection and property/performance requirements leads naturally to an interest in process-induced structural flaws along with microstructural features and their relationship to AM processing conditions. Materials engineers are likely to use CM tools to interrogate PSPP linkages that inform the AM Q&C process.

A suggested reading path is as follows:

- Section 3 Industry's Vision
- Section 4 Regulatory Considerations for CM Acceptance
- Section 5 Key Computational Materials Capabilities & Enabling Technologies
- Section 6 Key Elements & Associated Methods for Computational Materials Verification, Validation & Uncertainty Quantification
- Section 7 Computational Materials Simulation Maturity Level (SML) Assessment Framework

Researchers from mechanics, materials, measurement, manufacturing, and related disciplines should read the document to motivate and prioritize research and development (R&D) activities with the greatest potential impact on Q&C. The document should help researchers contextualize their work and identify opportunities to advance the state of the art in CM tools. The expectation is that the snapshot of the state of the art in modeling and simulation for Q&C reveals gaps in capability that inspire researchers to devise improved CM capabilities and new, more capable codes. This document should also provide context for such developments, showing how basic research can directly impact industrial needs.

A suggested reading path is as follows:

- Section 5 Key Computational Materials Capabilities & Enabling Technologies
- Section 6 Key Elements & Associated Methods for Computational Materials Verification, Validation & Uncertainty Quantification
- Section 7 Computational Materials Simulation Maturity Level (SML) Assessment Framework
- Section 8 Technology Maturation Path
- Section 9 R&D Investment Opportunities for CM Tools
- Section 10 CM Ecosystem Maturation

Software Developers should read the document to motivate product development in support of industrial adoption of CM tools. The document discusses gaps in the current commercial offerings. For example, most current packages lack tools for assessing uncertainty which is important for assessing the applicability of the results to real-world applications. The authors are aware that implementing such tools requires customer demand which is, of course, another aspect of this document. Software developers may find value in better understanding the aviation industry needs and the value proposition for translating CM methods and tools to industrial deployment.

A suggested reading path is as follows:

- Section 5 Key Computational Materials Capabilities & Enabling Technologies
- Section 6 Key Elements & Associated Methods for Computational Materials Verification, Validation & Uncertainty Quantification
- Section 7 Computational Materials Simulation Maturity Level (SML) Assessment Framework
- Section 8 Technology Maturation Path

Research and Technology Portfolio Leaders should find this roadmap beneficial for their understanding of the current state of CM as applied to AM and other manufacturing technologies, and a strategic pathway for the future of this field. These leaders are typically in industry and government laboratories with responsibilities for technology development and insertion. Others who are responsible for funding research and development, e.g., program managers in funding agencies, may find this document helpful as a community effort to define research needs for CM tools for Q&C and to assist in decision making regarding investments and organizational strategy.

A suggested reading path is as follows:

- Section 3 Industry's Vision
- Section 4 Regulatory Considerations for CM Acceptance
- Section 7 Computational Materials Simulation Maturity Level (SML) Assessment Framework
- Section 8 Technology Maturation Path
- Section 9 R&D Investment Opportunities for CM Tools
- Section 10 CM Ecosystem Maturation

Educators should find this document useful for understanding which topics are likely to be of most relevance to students or industry practitioners of advanced manufacturing, materials, mechanics, and measurement, or of greatest benefit in terms of skills to be learned.

A suggested reading path is as follows:

- Section 3 Industry's Vision
- Section 5 Key Computational Materials Capabilities & Enabling Technologies
- Section 6 Key Elements & Associated Methods for Computational Materials Verification, Validation & Uncertainty Quantification
- Section 7 Computational Materials Simulation Maturity Level (SML) Assessment Framework

Executive Summary

Although considerable scientific and technological advances have been made in recent years in additive manufacturing (AM) processes, these advances have not translated into significant market penetration of AM parts within the aviation industry. It is broadly acknowledged that using traditional qualification and certification (Q&C) approaches for AM components is one of the most significant barriers to broader adoption of AM, resulting in high costs, long product development and certification timelines, and complex design iterations during the product development cycle. A new approach is urgently needed. This document lays out a vision for a new Q&C paradigm with increased use of computational materials (CM) methods aimed at decreasing the time and cost of Q&C of process-intensive material (PIM) approaches in the aviation industry, with AM as the immediate use case. This vision was developed with substantial input from industry, regulatory agencies, government research organizations, and academia.

The discussion is built upon the foundation of an industrial vision for how CM approaches can be integrated into all phases of the new product development cycle, including not only its earlier phases such as material development, characterization, and design, but also the Q&C processes. Example business and engineering benefits include reduced time and resources for Q&C, improved part performance, streamlined insertion of new materials and processes, smarter testing inclusive of variations across parts, and improved focus for nondestructive evaluation resources. The cost and time benefits are based on incorporating emerging technologies to reduce the time to make informed decisions. Figure ES.1 summarizes the benefits of the digitally transformed future state for qualification as compared to the current state. The envisioned workflow leverages computational materials models that bridge the scales from material characteristics to engineering performance. This workflow will also lead to co-design of parts and process, i.e., each aspect influences the other in a bi-directional feedback loop, and will accelerate an *a posteriori* knowledge process to implement a digital transformation of engineering approaches. The strong business and engineering benefits of this approach leverage analysis and validated simulation results to efficiently supplement reduced physical iterations and testing. Expected gains from the approach include more-efficient utilization of resources, improved component performance through design flexibility, better understanding of the limits of the manufacturing and design spaces, and more streamlined adoption of new AM equipment and processes, among others.

Section 3 is followed by a discussion of regulatory considerations from the perspective of various certification authorities: the Federal Aviation Administration (FAA), Department of Defense (DOD) agencies, and the National Aeronautics and Space Administration (NASA). Subsequent sections of the document describe the key computational and supporting technologies that are needed to implement the industrial vision, and an assessment of existing capabilities and gaps in these areas. Simulation Maturity Levels (SML), derived from previous work on Tool Maturity Levels, are defined to provide standardized metrics for assessment and planning. We thus address slow adoption and acceptance of CM by the engineering community by encouraging quantifiable improvements in how computational materials science and engineering represents real world observed phenomena. The document concludes with a

detailed look at existing modeling, measurement, and ecosystem capabilities and needs, with a view toward providing the research community with an assessment of enabling research opportunities.

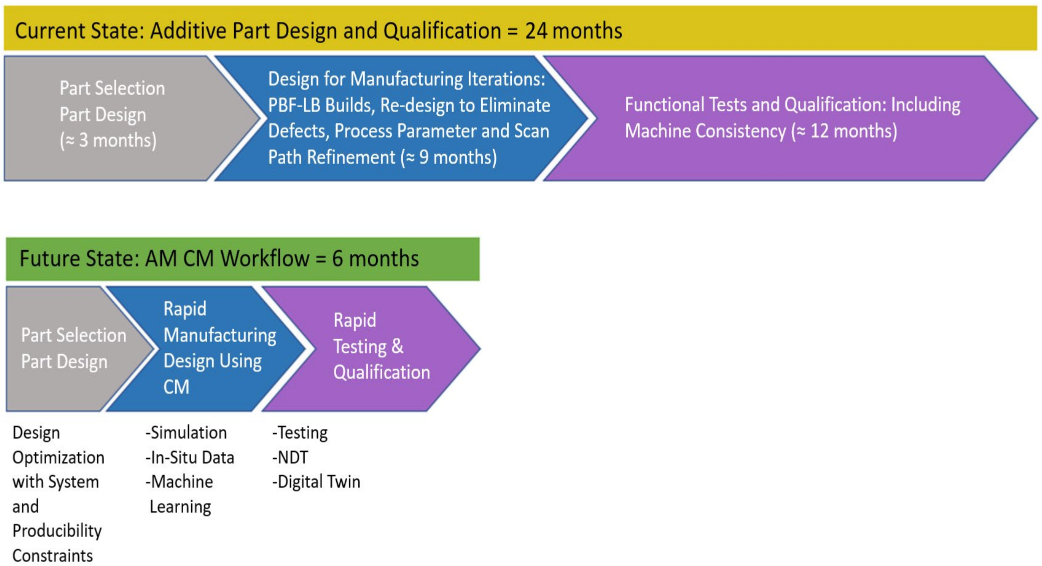

Figure ES.1: Summary of the projected benefits of the digital transformed future state compared to the current state for qualification.

Additive manufacturing processes, such as laser powder bed fusion (PBF-LB), offer a degree of control over the material and design that is unprecedented when compared with traditional manufacturing processes. However, the desired degree of control introduces enormous complexity, resulting in design risk compared to equivalent conventional product forms. The concept of understanding and quantifying process optimization to reduce variability and process uncertainty is an outcome of the AM CM workflow; understanding variability will efficiently establish repeatable and reliable materials and processes. When matured, this framework may challenge the conventional definitions and use of material allowables (which could be too burdensome given the degrees of freedom required for controlling AM process variation) to generate high-fidelity data, and to establish repeatable and reliable controls for an emerging design. The proposed framework thus provides a pathway towards understanding and controlling material and process variability, enabling a *smarter testing* approach where well-validated modeling results are supported by a meaningful yet reduced level of test data.

CM tools are already being used by engineers in the aviation industry at low technology readiness levels (TRL) for materials and process development to inform higher TRL technologies. These capabilities need significant maturation to enable industry to implement them at reduced cost, regularize their use, and incorporate them into Q&C packages with *design by analysis* as the prototype. The tools include those needed for process-structure-property-performance simulation with numerous multiphysics models at different time and length scales supporting various elements of this ecosystem. Deploying these tools for Q&C will require an investment in verification and validation (V&V) processes, along with uncertainty quantification (UQ). Both industry stakeholders and regulators should recognize the key aspects of verification, validation, and uncertainty quantification (VVUQ) in Q&C packages to build confidence that the combination of experimental data and simulation results constitutes a trustworthy approach. They should also be aware that the computational materials tools are in a heterogeneous state of readiness, which is the subject of a complete section in this report; certain areas, however, such as bulk residual stress predictions and computer coupling of phase diagrams and thermochemistry (CALPHAD), are at a high enough readiness level that they should be in regular use. Funding agencies should be aware that, inevitably, not all simulation techniques are at the appropriate readiness level for Q&C applications and this should be considered when supporting research to advance the CM codes and perform the required VVUQ. Industry and the U.S. Government have invested heavily in computational tools for materials processing, manufacturing, and properties prediction, yet these capabilities are currently accepted only in pre-Q&C phases of product development. To maintain U.S. competitiveness for both civilian and defense aviation applications, this document outlines a path toward updating the conventional (and largely empirically based) Q&C framework with well-validated CM-informed approaches that will accelerate the implementation of process-intensive materials approaches such as metals AM.

This work is also applicable to other manufacturing methods and applications (see Next Steps).

Section 1 Background

1.1. Introduction & Problem Statement

Whereas structural analysis is accepted as part of the qualification and certification (Q&C) process, the use of computational materials[‡] (CM) models has yet to be accepted in the Q&C domain because these capabilities are not considered to be sufficiently mature to be trusted by regulatory authorities and major original equipment manufacturer (OEM) product assurance and chief engineer offices. Consequently, current approaches used for qualification of materials and manufacturing processes are empirical (see, for example, Refs. [3–5]).

Nevertheless, the current technology and regulatory landscapes offer promise for development and acceptance of CM-informed approaches for Q&C. For example, the U.S. aviation industry uses CM approaches to support or guide the earlier phases of product development (e.g., material and process design). Additionally, the regulatory community currently allows for structural analysis "supported by test evidence" as part of Q&C (see, for example, Ref. [6]), with finite element structural analysis being commonly used in the certification process. Finally, as discussed later in this document, maturation of CM and required verification and validation (V&V) capabilities continue to evolve.

Understanding current accepted practices for development of new materials and processes and how qualification requirements are eventually determined is important for motivating and guiding the maturation of CM for Q&C. Today, when a new material or process is under initial development, desired attributes are estimated and then evaluated using selected, limited testing. This development, outside of the regulatory domain, is also typically supported by some level of integrated computational materials engineering (ICME) modeling. When feasibility to meet new material or process expectations is demonstrated by modeling, simulation, testing, and characterization (consider this to be in the approximate technology readiness level (TRL) 3-4 range), significant focused development – with the associated investment and extensive testing - can really begin. These efforts explore the material and process bounds for the intended part family application, and include physical, microstructure, and mechanical property characterization. Mechanical properties include those needed for preliminary design – like strength and stiffness – as well as those that affect creep, fatigue, and damage tolerance. In addition, potential flaw species for the material and process must be characterized, and the process limits and controls, chemistry, and microstructure ranges must be determined.

Scale up from laboratory-level sizes or configurations to representative full-scale parts must be demonstrated. Prototype parts will likely be manufactured by this point. Consider this to be approximately in the TRL 6/manufacturing readiness level (MRL) 6 range of maturity – where a system or program would have sufficient confidence to adopt the new material or process in a full-scale engineering and manufacturing development program for specific applications. This

[‡] *Computational Materials (CM)* is defined herein as the broad range of approaches for simulation of material processing, structure, properties, and performance (PSPP) that consider the underlying operative range of length / time scales and physical mechanisms. Additional definitions of key terms are available in Appendix VII.

would be equivalent to the beginning of full-scale product or system development for the general integrated product delivery process, or Milestone B [7] for Department of Defense (DOD) applications. Similar considerations apply to materials development and whether a new material is mature enough to be used in production parts. Recently, an approach based on materials maturity levels (MMLs) was developed[§], which is further discussed in section 8. The main point is that a material must have reached a sufficiently high MML to be considered for insertion into technology.

The development maturity at this point should be sufficient to finalize the material and process capability for all relevant requirements and properties – such as design *allowables*. These characterizations form the basis for *qualification requirements*, which would typically include formal specifications, manufacturing process specifications, purchase requirements, or even blueprint requirements for specific parts. Required acceptance criteria can be specified – for composition, microstructure, mechanical properties, and defect tolerances or acceptable anomalies. These may include specific testing and non-destructive evaluation (NDE) requirements, or other quality assurance requirements, which may be specific to individual parts and applications. The *certification requirements* then include the supporting documentation that demonstrates that the material and manufacturing process fully meet the qualification requirements and specifications.

Results of these efforts may be largely applicable and transferrable for use of the same material and/or process in other applications, with specific additional Q&C requirements imposed as appropriate for the application.

This explanation represents both the challenge and opportunity for a CM-based (or at least CM-augmented) Q&C process. For Process-Intensive Materials (PIM; see Section 1.2) like Additive Manufacturing (AM), the input material may go directly to a final (or near final) part configuration. Rapid iteration of design configuration and build process can readily be achieved, significantly reducing development schedule and cost. A robust approach to Computational Materials-informed Q&C, will enable the full opportunity space for AM, including location-specific microstructures, properties and performance parameters. To realize the full benefits and achieve broad implementation of AM and the broader PIM, the legacy processes of empirically-based Q&C must be dramatically improved. Of course, if a well-understood material is being used for AM, such as Alloy 718, Ti-6Al-4V, CoCr, Alloy 625, etc., prior data and AM process history may serve as a foundation. Nevertheless, individual AM machines, build practice, input powder, and part configuration will still require significant effort to achieve Q&C.

The proposed technologically updated CM paradigm will enable major improvements in time, cost, and extensibility of Q&C processes. While traditional Q&C approaches have served the

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[§] A. D. Rollett, M. K. Brinkley, P. E. Dimotakis, S. Graham, and V. Pugliano, Materials Maturity Levels: A Systematic Approach to Evaluating Materials Development, Integrating Materials and Manufacturing Innovation, (2025); doi:10.1007/s40192-025-00413-6.

industry and regulators well and have provided appropriate levels of product safety, such approaches are mostly empirically-based in the context of materials Q&C, and often do not provide adequate insights into the underlying physics relating the manufacturing process parameters, microstructure, properties, and performance. This lack of fundamental understanding makes process optimization, identification of the most critical process and material attributes, and quantification of the relationships between these aspects much more challenging. Furthermore, databases generated under test-driven frameworks are typically expensive, are highly process- and material-specific, and do not provide a feasible pathway for generalization or extrapolation to other similar material systems or manufacturing processes. These considerations are even more significant for new PIM technologies such as AM, resulting in a large number of manufacturing controls, a high level of process sensitivity, and a lack of in-service product and full-scale production experience.

A key feature of AM-built components relevant to Q&C is that the thermal history typically varies with location throughout the builds, producing components where the microstructures, compositions, and properties can be highly heterogeneous. Control and optimization of these local heterogeneities, along with assessment of the corresponding properties, could provide a significant advantage in the design, manufacture, and quality control of complex components by ensuring consistent performance and robust processes. In the longer term, capabilities for predicting location-specific material behaviors could drastically expand the design space.

Given this background, the CM4QC steering group has developed the following problem statement for this document.

Problem Statement: Utilization of CM-informed methods could greatly decrease the time and cost of AM Q&C in the aviation industry but requires a significant shift of both the engineering paradigm and the industry/regulatory culture [8,9]. The primary barriers to realizing these benefits are maturation and validation of required modeling and measurement capabilities and achieving acceptance by both industry and certifying agencies.

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

Increasing the use of CM capabilities for Q&C of metal AM is the key focus of this document. The key stakeholders and subject matter experts (SMEs) from the CM4QC steering group have discussed the corresponding business and technology drivers; the results are summarized below. It should be noted that this list is different from the similar ones in Section 2 and Section 3, with the latter being focused specifically on the key business and engineering benefits.

Business drivers

- Decreased cost and time of Q&C of AM components and systems
- Expanded design space for a given application offered for AM
- Expanded range of applications for both new systems and replacement parts for legacy systems
- 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
- Reduced product risk
- Democratized advanced manufacturing
- Transferability of knowledge between materials, machines, and parts

Technology drivers

- Advances, demonstrated successes, and increased use of CM, for example, the integration of CM in model-based engineering during the conceptual design phase
- Development of data standards, data interoperability, and digital enterprise (e.g., digital twins (DT), digital threads)
- Advances in high performance computing, artificial intelligence (AI), and machine learning (ML)
- Advances in V&V methodologies and maturation of credibility assurance frameworks (CAF)
- Advances in sensitivity and uncertainty quantification (UQ) 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

The following sub-sections (1.2 through 1.7) provide an overview of the key elements of this document that are relevant to the background discussion.

1.2. Primary Focus of this Document

The primary focus of this document is the introduction of CM approaches into Q&C processes for PIM technologies, as exemplified by metal AM. *For the purposes of this document*, a PIM technology is defined as an approach for producing products or parts that requires strict adherence to stable, detailed, and rigorous manufacturing processing steps combined in a fixed sequence, where any variations may have measurable effects on the material characteristics that in turn affect product performance. Examples of PIM technologies include AM, friction stir welding, and powder metallurgy. It is the degree of variation within the process, process complexity, and process robustness that determine its *intensiveness*. PIM represents a particularly impactful domain for CM applications, especially in the context of Q&C.

Although this document primarily addresses metal AM in the context of increasing the use of CM for aviation Q&C, this should be seen as a first example of this approach for the broader PIM and application space. The authors believe that most of the concepts, methodologies, and considerations discussed in this document are generally applicable to a range of PIM technologies and not just metal AM.

AM is re-invigorating metallic material design and deployment throughout industry. However, there is a growing realization that capability gaps exist for robust methods of compliance with existing certification requirements, particularly in fatigue-dominated high criticality applications. There is a significant lack of knowledge with respect to mechanisms of microstructure and flaw formation and their effects on properties and performance. Additionally, the large dimensionality of the process parameter space makes it both technically challenging and resource-intensive to characterize the variation in material properties and performance (e.g., fatigue response) for all possible combinations of process variables and local part geometries. Hence, a well-validated and uncertainty-quantified CM-based approach is envisioned as a path toward more-efficient Q&C methodologies that will further enable realization of the benefits of AM, including applications where conventional Q&C approaches are being challenged, e.g., for materials having spatially varying microstructures and compositions.

CM is a broad area of research and development (R&D) that employs computer-aided modeling of material Process-Structure-Property-Performance (PSPP) relationships, including the prediction of mechanical, physical, thermal, and chemical properties. It relies on integration of multiple disciplines including materials science, solid mechanics, fluid mechanics, thermodynamics, condensed matter physics, chemistry, computational mechanics, and experimental mechanics, among others. These capabilities have largely been applied to support material design, optimization, and processing (see, for example Refs. [10,11]), but have had little if any previous application in Q&C.

The confluence of a growing realization of the limitations of current approaches for Q&C of AM with the rapid maturation of CM capabilities inspired a recent Technical Interchange Meeting (TIM) on Computational Materials Approaches for Qualification by Analysis [8]. The TIM was co-organized by the National Aeronautics and Space Administration (NASA), the National Institute of Standards and Technology (NIST), and the Federal Aviation Administration (FAA) and was held at the NASA Langley Research Center on January 15-16, 2020. Approximately 60 SMEs representing 8 aerospace manufacturers, 8 government organizations, and 2 universities participated. Expertise of the SMEs spanned the TRL scale from the low-to-mid TRL focus of government laboratories and universities to the high TRL perspective of the aerospace manufacturers and regulatory organizations. During this TIM, the future needs of the manufacturers and government regulators motivated the overall discussion and framed the input given by the participants. Hence, the key objectives of the TIM were to understand existing gaps in model-based engineering (e.g., computational materials, processing and performance predictions) for aerospace materials and components and forecast how they can be matured to support material, process, and part-level Q&C.

One of the key recommendations that resulted from the TIM was to develop an integrated maturation plan for technology developers, educators, end users, and regulators with focus on incremental tangible progress and demonstrable deliverables [8]. The CM4QC Steering Group and this document were developed to address that recommendation.

1.3. Government Sponsored CM Efforts, Initiatives, & Software Capabilities

Numerous government-sponsored CM efforts and initiatives have been undertaken during the past two decades, including both general CM efforts and ones specifically focused on AM applications. Several prominent examples are described in Appendix I, Examples of Government-Supported CM Efforts, Initiatives, & Software Capabilities. The U.S. Government has also invested heavily in developing CM software capabilities that have become publicly available. Although the most pervasive investments have been made at various Department of Energy (DOE) and DOD labs, recently there has been increased effort at other government laboratories and by industry. Numerous foundational, often open-source, codes have been developed and used in a number of successful applications. Some examples of well-known publicly available CM codes[**] that have recently been used for AM are described in Appendix I, Government-Developed CM Software Capabilities. These prior efforts do not extend to the Q&C domain, whereas, this document aims to set the stage for such developments by government, industry, and academia for aviation Q&C.

1.4. Current use of Computational Materials-Related Capabilities

Appendix I lists examples of open-source codes that provide tools for researchers who are able to utilize software tools with minimal support. To meet the needs of industry users, however, commercial code suppliers typically offer support and consultation far beyond that associated with research codes. The state of the practice of the simulation tools is reviewed in Section 5 in enough detail to allow the reader to understand what is currently feasible. Other sections are more forward looking in terms of expected or desired advances in capability.

1.5. High-Level Lessons Learned from the Development & Introduction of Residual Stress Finite Element Analysis

As described in Section 1.2, the primary focus of this document is the maturation and broader acceptance of CM approaches into Q&C processes for PIM technologies, as exemplified by AM. It is useful to look at historical precedents in related fields to see if valuable lessons may be learned that could provide guidance to the current focus. Appendix V explores the history and modern development of residual stress simulation using finite element analysis (FEA). Several high-level lessons can be learned from this field, including the vital importance of:

- Code verification
- Model validation against rigorous (e.g., benchmark) measurement data
- UQ for both measurement *and* modeling results
- Incorporating CM approaches into the qualification process

When implemented correctly, these approaches have demonstrated significant time and cost reductions in related industrial segments, as well as durability and safety improvements.

[**] Certain equipment, instruments, software, or materials are identified in this document in order to specify the experimental or analysis procedure adequately. Such identification is not intended to imply recommendation or endorsement of any product or service by the U.S. federal government, nor is it intended to imply that the materials, equipment, or software identified are necessarily the best available for the purpose.

1.6. Importance of Verification, Validation, & Uncertainty Quantification

In contrast with experimental data that typically includes error bars and confidence intervals, CM results often do not. This deficiency makes it difficult to base decisions on CM, especially high-consequence decisions such as the Q&C of critical parts. Achieving a level of confidence in simulations that allows them to inform decisions requires thorough V&V of models, along with an understanding and quantification of the sources of model uncertainty. Verification of codes and solutions ensures that the model is being solved correctly and that the amount of numerical error is bounded and of an acceptable magnitude. Validation assesses the model's ability to accurately simulate reality; this evaluation must be based on experimental data. Sources of model error assessed by validation can include unknown or variable parameters and conditions, as well as inaccuracies in the assumptions or mathematical form of the model itself. UQ consolidates knowledge of the various sources of numerical and model error to calculate how they propagate through the model to the simulated quantities of interest (QOI). Where possible, UQ may be used to compute the expected probability distribution of the true quantity predicated on the available experimental and simulation data. An overview of key enabling technologies for CM, including validation measurements, ground truth characterization, and UQ theory, is given in Section 5 of this report, while a more detailed discussion of V&V and UQ for CM models is given in Section 6.

Improving the state of V&V and UQ for CM tools should be a concerted effort by software developers, experts in computational materials and mechanics, experimentalists, and other stakeholders. In Section 7, a framework is outlined for assessing the Simulation Maturity Level (SML) of CM capabilities, including criteria for evaluating the status of V&V and UQ. It is a goal of this document to help educate stakeholders in the aviation industry about the feasibility and importance of UQ, because only industry's recognition of this necessity will ultimately drive commercial software developers to fully integrate UQ into their products. It is worth noting that the American Society of Mechanical Engineers (ASME) VVUQ-10 subcommittee on Verification, Validation, and Uncertainty Quantification in Computational Solid Mechanics explicitly states that a successful V&V process is impossible without the elements of UQ.

1.7. Key Terms

Several foundational terms are critical for understanding the main themes of this document. In particular, *Computational Materials* (CM) is herein defined as the broad range of approaches for simulation of material processing, material structure, and/or material properties and performance. *Integrated Computational Materials Engineering* (ICME) involves coupling of CM tools to accelerate materials development and unify design and manufacturing (adapted from [10]), the degree of tool integration and coupling being a distinguishing factor. The CM4QC steering group is primarily focused on the structured application of CM specifically to inform Q&C activities, i.e., Computational Materials-informed Qualification and Certification. This may involve toolsets and workflows categorized as ICME, however the specific application to Q&C objectives is an important distinction with significant practical impact, as detailed in the remainder of this work.

The terms Qualification and Certification are used throughout this document, either individually or in tandem (i.e., Q&C). While an interpretation of each of these terms (*in the context of this report*) is included in the Glossary (Appendix VII), it is recognized that there are multiple interpretations in use across the industry and government agencies. For the purposes of this document, a simplified interpretation is that qualification refers to a set of engineering activities performed by a company, while certification is a formal and highly regimented process that is governed by existing regulations and therefore is specific to a particular regulatory agency. At the same time, a number of the underlying technical considerations for both qualification and certification may be quite similar, both aimed at ensuring the development and manufacture of a high-quality and safe aviation product. Most of the detailed technical considerations relative to the expanding use of AM are formulated in the context of the *qualification* process. While we expect that many of these considerations will be equally applicable to the use of CM in the *certification* process, a more detailed guidance would need to be developed in close coordination with the appropriate regulatory agency to cover this topic (also identified as a next step in Section 11). Such development may be a subject of a follow-on activity, after the publication of the current document.

Lastly, it should be noted that the important term *defect* is used very differently in different fields and may cause confusion. In physics and materials science, *defect* refers to any localized disruption of a perfect crystalline order. Thus, a single interstitial atom is referred to as a point defect and a single dislocation is referred to as a line defect. In contrast, in engineering practice, a *defect* is defined as a *flaw* whose size, shape, orientation or location makes it detrimental to the useful service of its host object or exceeds an accept/reject criterion of an applicable specification. A *flaw* is then defined as an interruption, imperfection, or irregularity in the physical structure or material state of a part or a specimen. In this document, when the term defect is used without a modifying adjective, it should be assumed that the practical engineering definition is being used.

Appendix VII provides additional definitions of key terms utilized throughout this document. Where possible, these definitions have been adapted from prior work for consistency.

1.8. Laser Powder Bed Fusion as a Use Case, and its Relevance to other Forms of PIM

A large majority of published metal AM research has focused on laser powder bed fusion (PBF-LB), the build method that is most heavily used for aviation applications. This makes PBF-LB a good PIM use case for CM4QC's initial focus. While much of the discussion in this document is similarly focused on PBF-LB, the underlying mechanisms and PSPP relationships are relevant to a much wider range of AM build methods. Also, the proposed CM4QC framework is largely agnostic to the specific PIM approach. Thus, the framework descriptions and conclusions, based on the selected use case, are relevant to a wide range of AM and broader PIM methods.

Section 2 Scope

2.1. Introduction

This document is intended to identify key considerations and enablers required for maturation and broader acceptance of CM approaches into aviation Q&C processes. This goal will require advancements in high-fidelity modeling and simulation along with methods for verification, validation, and uncertainty quantification (VVUQ) to a level adequate for the certifying authorities' and OEMs acceptance of the use of CM methods as a key part of Q&C of structural or flight-critical PIM parts. In the next sub-section, we summarize (in bullet form) the key objectives of this document along with the desired impacts and relevant gaps.

2.2. Key Objectives for this Document

The overall goal of this document is to develop a pathway towards a CM-informed Q&C framework for PIM technologies to be used by aviation industry and government regulatory agencies and enabled by basic and applied research. This goal is supported by the following key objectives and desired outcomes:

- Detail the current state of Q&C for PIM parts.
- Document industry vision for the use of CM in qualification.
- Identify regulatory considerations for the use of CM in certification.
- Identify key considerations and enablers required to increase airworthiness of AM components and certifying authorities' acceptance of computational methods.
- Assess current CM tools and capabilities, including for VVUQ, across industry, government, and academia, as well as the current state of use within the aviation industry.
- Identify current gaps and R&D investment opportunities associated with maturation of CM and supporting technologies.
- Develop a framework to evaluate the maturity level of CM simulations for potential use in Q&C.
- Initiate a paradigm shift in the aviation industry's use of CM tools.
- Encourage increased dialogue among the stakeholder organizations and promote collaboration and coordination among these organizations in the context of implementation.
- Encourage development of relevant guidance/standards from standards development organizations (SDOs) and relevant government agencies.
- Inform academia about training and education gaps.

2.3. Desired Impacts for this Document

The overarching envisioned impact of this document is the eventual adoption of CM tools into the Q&C practices of the aviation industry (and eventually other sectors).

Specific impacts include:

- Enabling coordinated execution of a multi-year maturation plan for CM in the Q&C domain
- Increasing standardization and best practices for CM-enabled Q&C for the aviation industry and government agencies (contributing to faster Q&C)

- Enabling industry and government agencies acceptance of CM approaches for Q&C of AM and other PIM processes
- Motivating corresponding investments by industry and government
- Expanding technical communication/coordination across the CM community of practice and its stakeholders, including workshops
- Inspiring new university courses and workforce education targeting CM for Q&C

Some of the key business and engineering benefits underlying these impacts are listed here and described in detail in Section 3.4. The numbers correspond to the corresponding Section 3.4 subsections.

1. Reduced time and resources for Q&C of high-consequence aviation components
2. Improved part performance through design flexibility
3. Accelerated development of tailored alloys for targeted AM applications
4. Development and acceptance of new AM machine architectures
5. Accelerated *delta qualification* of machines with minor hardware/software changes, and qualification of new sources using the same machines and software
6. Quantified and mitigated build variations
7. Implementation of smarter testing inclusive of the variation across the part
8. Use of AM build process and performance modeling to focus resources for non-destructive methods
9. Enabled rapid and confident decisions for disposition of manufacturing non-conformances in production
10. Q&C decisions based on performance risk enabled by CM engineering

2.4. Gaps Limiting CM Maturation & Adoption for Q&C

Lastly, it is useful to list current gaps that limit both CM maturation and its adoption for Q&C applications. These gaps include, but are not limited to:

- Insufficient maturity of CM and associated tools for use in Q&C activities
    - A maturity assessment of such tools is provided in Section 9 and Section 10
- Inadequate metrics for assessing the maturity of CM tools for use in Q&C activities
    - Section 7 addresses this lack by introducing an SML assessment framework
- Lack of acceptance by regulatory agencies and industry (beyond R&D and material/process development)
    - Overcoming this issue will involve a paradigm shift in the direction of design-by-analysis, including hiring new employees trained in the use of these technologies and adding to the skillsets of existing employees. Internal roadmaps will be needed to outline implementation points in the development process, including V&V strategies. Progress in this direction will necessarily be incremental.

    - Development of product-specific business cases and trust in models are key requirements. A business case may include reduced cycle time and development of more advanced and reliable designs. Acceptance of a CM-informed approach to Q&C must start with small, well-defined steps that are visible to the organization and will deliver tangible interim benefits. Increasing the model trust can be achieved through the effective application of V&V or CAF.
- Lack of publicly available validation measurement data
    - Model validation measurements are distinctly different from more traditional discovery experiments, and data availability is limited. Most validation data used by OEMs for Q&C is proprietary. One example of a source for publicly available AM model validation data is the Additive Manufacturing Benchmark Test Series (AM Bench) [12,13].
    - The biggest hurdle may be lack of data having a suitably rigorous provenance; hence data generated for other reasons should be evaluated, curated, and made available for reuse. FAIR data principles (findability, accessibility, interoperability, and reuse of digital assets) should be adhered to whenever possible [14,15].
    - V&V is discussed in Section 6 and Section 7.
- Limited capabilities for UQ of CM simulations
    - Surrogate models might play a major role in this area since they tend to be much faster than full-scale physics-based models.
    - The current state of UQ for CM simulations is discussed in Section 6.
- Lack of consensus approaches and standardized methods for Q&C
- Insufficiently prepared workforce for the expanding use of CM

All of these gaps will be addressed within this document.

Section 3 Industry's Vision (for Q&C and other foci)

3.1. Introduction

Materials and process innovation is key to revolutionizing the U.S. economy. In the same way that silicon in the 1970s led to the modern information technology (IT) industry, the development and adoption of advanced materials and manufacturing approaches will allow us to address challenges in aerospace, energy, national security, healthcare, and other areas [11]. For the aviation sector, many ground-breaking technologies have been recently introduced that will significantly transform aircraft performance, durability, and efficiencies, as well as the manufacturing base. The development and adoption of novel materials and manufacturing processes, like metal AM, have increased U.S. competitiveness by spurring new markets and business opportunities for the manufacturing sector, increasing robustness of the supply chain, and enhancing the ability of companies to create novel products through more optimized designs.

However, the adoption of these novel technologies can be hindered by concerns about repeatable and reliable performance and quality. The resulting enterprise-level digital and operational transformation efforts to modernize the manufacturing base have produced a complex landscape with unique ecosystems. CM engineering approaches have recently gained popularity as a solution to these challenges through accelerated adoption of new AM materials and processes for aviation companies.

The aviation industry continues to rely upon legacy solutions based solely on comprehensive experimental testing for new material or part qualification, or the certification of a new material or part by a regulatory agency. Meanwhile, the use of ICME in an industrial setting has grown over the past several decades from an academic novelty to a set of standard processes and tools that have been found to accelerate the development and insertion of new materials and processes [10]. It is essential to note that adoption of CM engineering on an industrial scale depends on several factors, including not only technological advancements, but also cost-effectiveness, regulatory frameworks, workforce development, and market demand. While the industry has made significant progress, further advances are necessary to realize the full potential of these technologies.

The industry vision is to reduce the time and cost of introducing high-criticality AM-processed aviation components while enabling the introduction of new materials and more-efficient part geometries. This high-level vision aligns with United States Congressional sentiment of concern over the aging U.S. manufacturing base and its diminishing infrastructure. The emergence of PIM approaches like AM presents a remarkable opportunity to revive this sector and reestablish a competitive global presence. By embracing CM engineering approaches, the U.S. can unlock new possibilities, drive economic growth, and regain its leadership position in manufacturing. With continued investment, these CM-informed tools for Q&C could develop to match the current maturity of computational analysis tools in the design space. As the CM tools and processes become better vetted and predicted outcomes become trusted for a variety of materials and processes, a more competitive and effective economy can be realized.

3.2. Opportunities & Challenges for CM Engineering & AM in Aviation Industry

The traditional *economies of scale* operation models have driven manufacturing success by enabling repeatable and reliable mass production. However, novel technologies like AM offer a paradigm shift, greatly expanding manufacturing possibilities and emphasizing *economies of scope* operation models. By utilizing AM techniques, manufacturers can create customized designs that are highly optimized in both their spatial configuration and their material composition within a single production process. This capability enables companies to enter new markets, reduce costs associated with product varieties, and unlock untapped potential. CM engineering further enhances economies of scope by optimizing material properties and performance, ensuring superior quality and functionality of printed parts.

Today, there are many uses of CM tools in the early stages of the new product development cycle, including material design, or process design, to explore regions of promising chemistry or process space that can then be tested in a traditional manner. This approach assumes that models exist that can appropriately predict the resultant microstructure and properties from the initial chemistry and manufacturing process. While this assumption may hold true for well-understood materials within a defined chemistry and process space, extrapolating outside of the initially validated bounds of these models can result in significant error. CM modeling can evaluate the impact of small deviations from the ideal chemistry or process, but large changes outside of the validated range still require significant testing to demonstrate accuracy and quantify uncertainties. Generating comprehensive allowables data for a given material and process is expensive in terms of time and effort (> $1M and > 18 months) [16].

Revolutionary design advancements in aviation components are one of the key business cases of AM. The traditional lead-time for manufacturing a new, complex component is drastically reduced, as is the cost for small volume and single-part production. Additionally, reduced part weights, subassembly part counts, and inventories are also realized. All these benefits have driven the aviation industry to consider how to accelerate the adoption of this novel manufacturing method, not only in prototyping but also in the AM of high-criticality components [17].

One challenge to the adoption of additively manufactured components lies in the quality control of not only the AM machines themselves, but also the quality system that surrounds the entire component manufacturing ecosystem, including feedstock materials such as powder or wire, build atmosphere, shop practices, maintenance, inspection, subsequent thermal or surface processing, etc. The key to faster adoption in today’s market has been to create robust quality control and qualification procedures that can produce a consistent, uniform material state with statistically reliable material properties, which translate into trusted material allowables. In addition, a clear interpretation of certification requirements is needed in order to demonstrate to any certifying agency that the appropriate steps have been taken in analysis, especially for high-criticality components. CM tools are expected to play a key role in addressing some of these challenges related to Q&C.

By applying a CM-based engineering approach, the variations in the AM process could be simulated to understand the resultant variations in microstructure, flaw state, properties, and performance. A robust CM tool suite for AM could help the aviation industry better understand the impact of different aspects of the quality control process on the final material allowables and product durability. To fully vet the process models for this novel manufacturing method, the development of in-process monitoring methods on additive machines is required to better validate the connection between what the machine is programmed to do versus what is actually happening within the build. In-process monitoring offers the potential to connect actual process conditions with the CM process models in real time (or near real time) to ensure an AM build will meet intended quality and performance requirements locally – for every part. This also offers the opportunity to base acceptance criteria on a suite of parameters, and to provide feedback for process and model improvement over time. These attributes offer the potential to improve a process well beyond what a legacy *frozen process* approach would yield. Additionally, appropriate nondestructive testing (NDT) techniques are needed to assess the material in the as-built and final production configuration to understand the level of any inherent material anomalies such as porosity. This knowledge is required to build the appropriate process models and to use them to help set the appropriate limits of a production process. Thus, in-situ and ex-situ inspection data should be fed into an appropriate CM framework for Q&C of the printed components.

One of the biggest challenges to applying CM engineering more broadly is the need for understanding error propagation across the time and length scales. Any validation process must consider the impact of the required inputs to the model and the uncertainty in the measurement of those initial inputs. If the CM tools are to support the development of the design data for certification, then the validation process must consider not only the variation due to the manufacturing process, but also due to the error associated with model uncertainty. Even when the resulting uncertainties are too large to produce a reasonable material allowable, the validation process may still be extremely useful for understanding the impact of process variations and for reducing the number of iterations of a process design before obtaining an optimum configuration. The benefits, requirements, and general approaches for model validation are discussed extensively throughout this document, especially in Section 6.

3.3. Roadmap for Development & Adoption of CM Engineering Tools

The vision for the future state of CM engineering approaches for AM applications should prioritize attainable and practical intermediate outcomes, or off-ramps of applicability, to drive successful development and enable confidence in various aspects of the process. Development of such off-ramps can be best achieved by focusing on well-understood alloys such as Ti-6Al-4V and Nickel Alloy 718 to establish confidence in the use of CM in the Q&C domain and establish a standard framework across the industry. These materials serve as a solid starting point for the development of PSPP models.

A possible near-term off-ramp could involve creating a standardized SML for the PSPP models and simulations. A proposed SML framework is presented in Section 7. This process includes thorough assessments of UQ and V&V methods, ensuring the reliability and consistency of the models within an established range of applicability. Establishing such SMLs would foster confidence in the CM engineering approach and set the stage for further advancements.

In the mid-term, a possible *off-ramp* would be the expansion of these models to cover a broader range of widely used materials. These models would enable assessment of the impact of process variability and intentional or inadvertent process changes on design allowables. By implementing these models for familiar materials, we can gain valuable insights into the effects of different process variations and adapt accordingly to enhance component design, performance, manufacturing workflow productivity, and yield.

Looking towards the long-term, another significant *off-ramp* goal would be to leverage related ICME tools to develop new alloys based on design requirements and predict the performance of components built with the newly designed alloys as a function of processing conditions. This may necessitate the establishment of reduced/rapid testing protocols for validation, allowing confident exploration of new manufacturing frontiers and adoption of innovative materials and processes. Analogous to these material maturity-based off-ramps, CM-informed Q&C would support insertion of these alloys with progressively increasing part criticality, i.e., from non-critical to critical parts.

By strategically following this approach, CM engineering can progressively advance in the Q&C domain. While the goal of significantly changing the balance between the use of test data versus models in the Q&C domain remains ambitious, incremental achievements in creating standardized models, expanding material coverage, and venturing into novel chemistry and processes will drive us closer to that vision. Through collaboration and collective efforts, we can usher in a new era of materials engineering, unlocking unprecedented possibilities for industry-wide advancement.

One key and fundamental challenge will be how to determine and validate the level of *transferability* or reuse of the various CM modeling efforts. The cost of model development and VVUQ for CM approaches to ensure suitability for qualification and certification will be significant. It will not be successful if every application requires a full suite of VVUQ. Certainly, for the same material (meaning base alloy and processing), for the same models or suite of models, for applications within the same or similar part family, or within similar applications – there must be a process to assess the level of transferability.

Figure 3.1 illustrates the vision for a future state of CM engineering, in which a comprehensive balance of testing and analysis would be seamlessly integrated into various stages of the design process. This comprehensive approach that incorporates CM at its base, would span the range from raw materials, through component, sub-assembly, and ultimately final system configuration. Throughout these levels, both *physical* test data and *virtual* or model-generated data would synergistically inform the design, manufacturing, and materials teams. The virtual data from the well-calibrated models provides valuable insight in predicting the trend in the QOI. Physical data would be used to calibrate the model to improve the fidelity of prediction. The extent of reliance on *physical* versus *virtual* data would be adjustable, based on the fidelity of the models and the cost/benefit considerations in enhancing that fidelity. The envisioned future state enables the integration of model predictions with complementary test data [18]. Consequently, the development time and cost associated with novel manufacturing methods, materials, and their integration into aviation components and systems could be substantially reduced [19–21]. This harmonious interplay between physical testing and advanced modeling empowers the aviation industry with valuable insights and improvements in efficiency and effectiveness. By harnessing the strengths of both approaches, industry can expedite innovation, optimize design processes, and drive significant advancements in aviation technology.

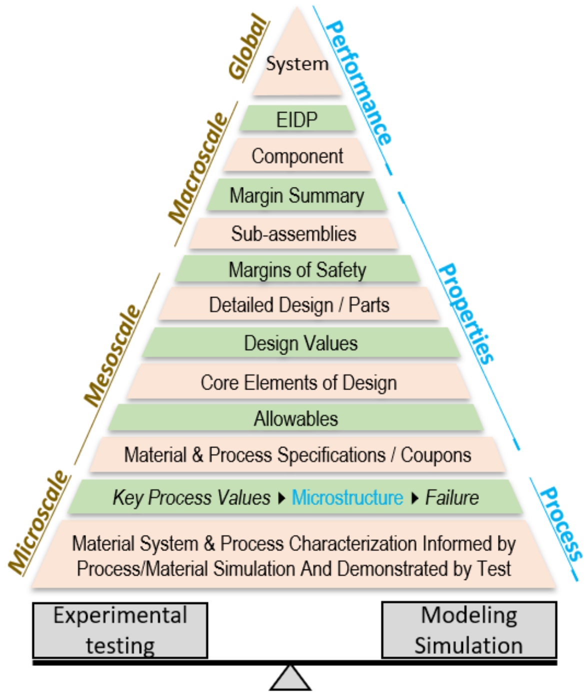


Figure 3.1 Future state of product development with optimized CM + experimental approach. Orange boxes in the pyramid correspond to the elements at different length scales and the green boxes are associated data linking the adjacent length scales, with the end item data package (EIDP) at the top. The bottom graphic indicates a balanced approach for experimental testing and modeling simulation.

In comparing the current and envisioned future states of qualifying and certifying additively manufactured aviation components, a significant difference in approaches can be observed. Figure 3.2 shows the current state of the framework employed for qualification of components in the aviation industry. It depicts the multiple stages involved in the current workflow from requirement specification to (pre-certification) qualification of the component. The workflow starts with system/sub-system requirements. Based on the specifications, the component will be designed with appropriate material selected and analyzed virtually using computational methods (structural analysis). This design step is followed by development and qualification of the process to fabricate the designed component. Allowables data for the chosen material system fabricated using the qualified process are then generated. The component is fabricated and inspected using appropriate NDE methods followed by overall qualification of the component. Currently, except for multi-physics design analysis (structural analysis), all the other stages in the workflow are dictated by experiments with physical iterations at individual stages as needed. To fully grasp the impact of material anomalies or property variations across the part, physical manufacturing, inspection, and testing of components are essential to provide crucial feedback to the design process with these physical iterations. This current approach, while proven to be reliable for a variety of material systems, comes with notable time and resource demands, leading to a slowdown in the qualification of aviation components. This is particularly true for AM, where local processing conditions may vary with location throughout AM builds, as well as between builds, producing components where the local microstructures and properties can be highly heterogeneous. Traditional coupon testing is of little value if the structure and properties of the coupons are not representative of the components that must be qualified and certified [22].

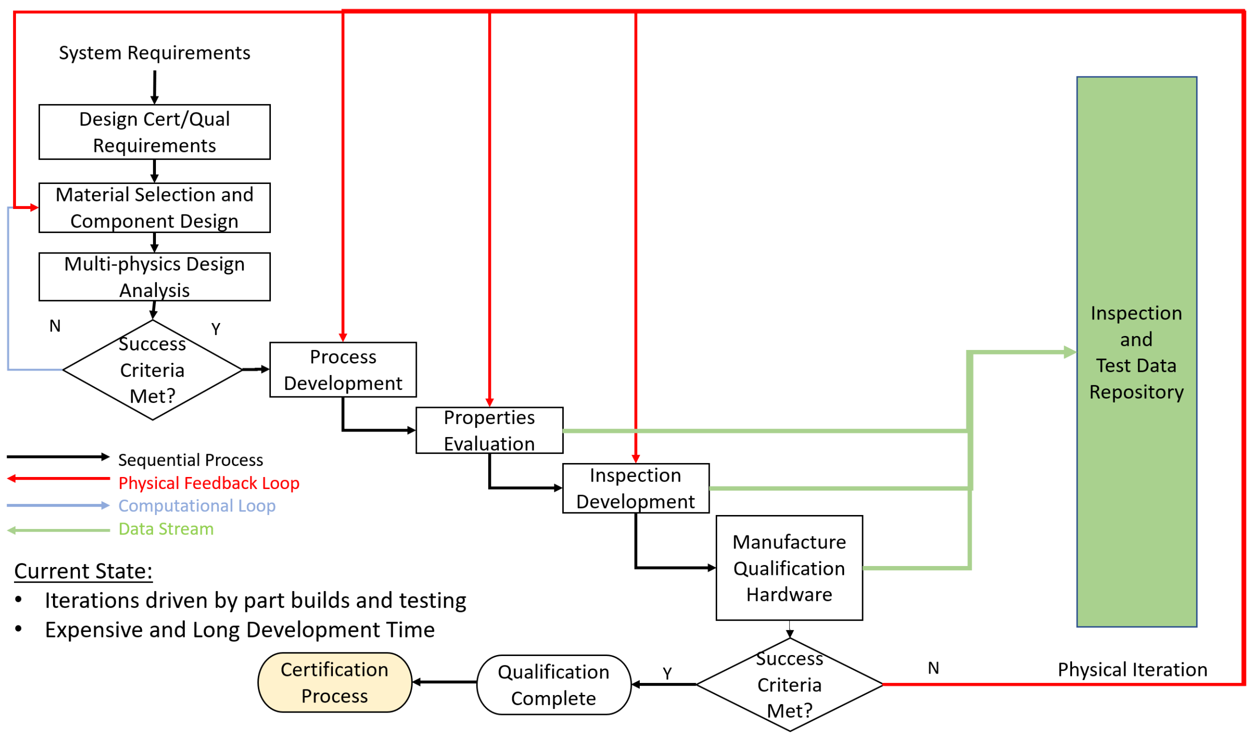


Figure 3.2 Current state of qualification of components (pre-certification).

Recognizing this challenge, the industry is evaluating various options including transitioning towards a future state that embraces more advanced CM engineering techniques to streamline the Q&C process by augmenting testing with simulation [23]. In the proposed approach (Figure 3.3), mature CM and UQ tools are introduced at each stage of the traditional workflow. This diagram demonstrates the proposed integration of CM into the broader context of material and component design and qualification. With the use of computational iterations throughout the workflow, the required experiments can be intelligently designed, resulting in cost and time reductions. The key point is to utilize mature (validated) CM tools. Various steps involved in maturing a CM tool for a given stage in the workflow is shown in the box labeled “CM Multi-Scale Model development” in Figure 3.3. It has 4 stages starting with designing the numerical methods, developing the model with appropriate physics, followed by model calibration and validation. Model calibration and validation processes should include sensitivity and uncertainty analyses associated with the inputs and outputs.

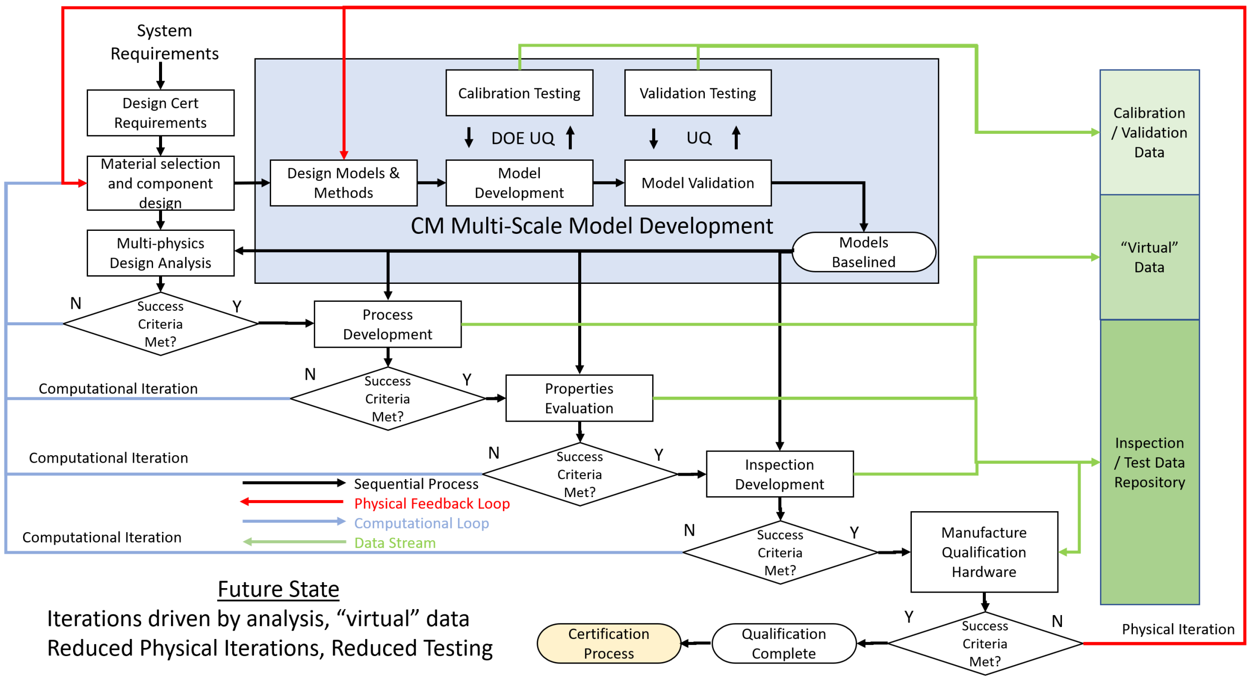


Figure 3.3 Future state of computational materials engineering informed qualification (pre-certification). Note that some steps are conducted on an as-needed basis and may not be required for every iteration.

By harnessing CM methodologies, a more-efficient and comprehensive understanding of material behavior and performance can be achieved, expediting the introduction of repeatable and reliable materials and processes vs. conventional qualification methodologies. The integration of advanced CM tools and predictive models promises to transform the qualification process, reducing the reliance on extensive physical testing and enabling a more agile and production informed decision-making framework. In this envisioned future state, manufacturers will be better equipped to assess material behavior, optimize designs, and validate performance supplemented by modeling and simulation. This shift towards a simulation-driven approach represents a significant advancement in the aviation industry, ultimately accelerating innovation and ensuring the successful integration of novel materials and processes into critical aviation systems.

Embracing a CM approach, the PSPP models represented in the "CM Multi-Scale Model development" box (Figure 3.3) empower early design decisions by assessing the alignment of design, manufacturing processes, material properties, and inspection methods with success criteria for the component. The various modeling, measurement, and infrastructure components shown in this box are more thoroughly introduced in Section 5.

At every stage of the process, valuable virtual data are captured and stored in a comprehensive database. This repository includes initial physical calibration and validation data used to create the CM models, as well as subsequent physical inspection and test data obtained after producing several initial components. This data-intensive approach significantly reduces the number of physical coupon and component builds required, effectively minimizing testing efforts.

The crux of this approach's success lies in the predictive capabilities of the CM models within the specified range. To gain acceptance as an acceptable method of compliance from certifying agencies, comprehensive data analysis is essential to substantiate the methodology's reliability and accuracy. Adopting this advanced CM-driven approach empowers engineering teams to make well-informed design decisions early in the process, streamlines testing efforts, and optimizes the Q&C of aviation components with novel materials and processes, including AM. Consequently, this approach paves the way for more-efficient, cost-effective, and reliable aviation manufacturing practices, propelling the industry towards cutting-edge and groundbreaking advancements. Some examples of key business and engineering benefits of the envisioned future state (Figure 3.3) are further discussed in Section 3.4.

3.4. Business & Engineering Benefits of AM CM Engineering to Industry

The envisioned future state, driven by the adoption of a CM engineering approach for AM Q&C, presents numerous key business benefits.

1. Reduced time and resources for Q&C of high-consequence aviation components
2. Improved part performance through design flexibility
3. Accelerated development of tailored alloys for targeted AM applications
4. Development and acceptance of new AM machine architectures
5. Accelerated *delta qualification* of machines with minor hardware/software changes, and qualification of new sources using the same machines and software
6. Quantified and mitigated build variations
7. Implementation of smarter testing inclusive of the variation across the part
8. Use of AM build process and performance modeling to focus resources for non-destructive methods
9. Enabled rapid and confident decisions for disposition of manufacturing non-conformances in production
10. Q&C decisions based on performance risk enabled by CM engineering

The following subsections detail the business and engineering benefits outlined above.

3.4.1. Reduced Time & Resources for Q&C of High-Consequence Aviation Components

Utilizing a CM engineering framework, even simulations with a relatively modest SML of 3 offer significant advantages in guiding and expediting experimental trials across materials design, process development, and product development cycles. Linked PSPP models play a crucial role in evaluating how key process parameters impact the microstructure and final properties of the manufactured part. To address uncertainties and variations in inputs, a model uncertainty analysis is executed, quantifying and demonstrating corresponding uncertainties and variances in the outputs. The model-based UQ approach effectively captures variations in final part properties across different locations and assesses property sensitivities to uncertainties related to process parameters such as temperature, laser power, and speed. By conducting model-based sensitivity analysis of process parameters to resulting properties, engineers can develop robust process controls to ensure part properties meet desired design requirements. Implementing these methodologies expedites the acceptance of similar machine sources or parameters that are not identical and accelerates root cause investigations when process parameters have been modified or drifted unknowingly.

As an example of established CM tools that could be matured for use in Q&C activities, the use of thermo-kinetic models (including computer coupling of phase diagrams and thermochemistry (CALPHAD) approaches with diffusion kinetics) for nickel alloys provides insights into the impact of gamma prime precipitate stabilizers on AM layer properties, such as propensity for crack nucleation. By adjusting the composition of these stabilizers, it becomes possible to design an alloy with improved printability, reducing the number of Design of Experiments (DoE) sets required to fine-tune the alloy composition. In the case of alloy design for turbine engine disks, forging models integrated with disk growth models optimize the disk design microstructure, reducing residual stresses and disk growth in critical locations [24]. Combining this optimization with model-based UQ enables precise definition of material specifications and tolerances for a new disk design. This approach determines the level of quality control needed during the disk manufacturing process, eliminating the need for several production trials to establish a stable operating process window.

Leveraging CM-driven approaches empowers engineers to efficiently design and manufacture high-performance components with enhanced predictability and optimized properties. By integrating computational materials models, uncertainty analysis and sensitivity studies, the engineering process becomes more robust, reducing development cycles and leading to reliable and high-quality aviation components.

3.4.2. Improved Part Performance Through Design Flexibility

CM engineering is a transformative approach that seeks to integrate CM tools into a comprehensive system, revolutionizing materials development and streamlining engineering design optimization. By bridging the gap between design and manufacturing, CM engineering aims to achieve closer-to-optimal designs with respect to cost, weight, performance, and other critical factors. In traditional design and manufacturing practices, achieving optimal designs often requires multiple costly and time-consuming iterations in material processing and part configurations. However, with the implementation of model-based engineering, the design process becomes more efficient, and the number of physical iterations is significantly reduced, while simultaneously producing designs that are closer to the optimum. CM engineering plays a crucial role in providing valuable insights to part designers by offering a deeper understanding of potential variations in material microstructure and properties within a component. Equipped with this knowledge, designers can optimize component designs through manual or automated iterative processes, considering the resultant structure and properties influenced by the component’s shape. CM capabilities can also support Design for Manufacturability (DfM) by providing insights into manufacturing process robustness as a function of chosen part design.

The application of CM engineering is particularly advantageous in AM. In this context, designers can consider not only the component’s geometry but also manufacturing process variables, such as scan patterns, layer thickness, support structures, and other parameters. This holistic approach empowers engineers to optimize designs that account for both the final dimensions and the manufacturing process, leading to enhanced component performance and more-efficient use of materials.

Ultimately, the integration of CM engineering into design optimization promises substantial benefits, including reduced component weight, lower fuel consumption, and overall lower life cycle costs in engineering and manufacturing processes.

3.4.3. Accelerated Development of Tailored Alloys for Targeted AM Applications

In the development process of new alloys, ICME approaches can be employed, provided that the models used can accurately capture the relationships between the manufacturing process, microstructure, and critical design properties. The key to successful implementation is to ensure that the models operate within the applicable chemistry range, as extrapolating beyond the validated regions may lead to unreliable predictions. Within the validated range, these models can generate *virtual* data, which when combined with actual test data, can significantly reduce the overall testing burden during the development program. In addition, these models have the potential to reduce or eliminate development iterations, and to reduce the impact of such iterations by reducing the time and testing required to execute and iterate. The value of this benefit depends on whether the validation data for the model is more or less expensive than the reduced amount of testing required. The benefits further increase if the modeling approach can effectively minimize the testing needed to verify inadvertent or intentional process changes during production. This approach has been successfully demonstrated for a variety of new alloys designed for AM applications. One notable example is the development of a new AM-compatible steel for U.S. Army helicopter rotorcraft gears that combines improved bending and contact fatigue resistance, enhanced core strength with good toughness, higher temperature resistance, and excellent hardenability [19,20]. Another notable example is designing high strength AM aluminum alloys for high temperature applications (200 °C to 400 °C)[25–27]. These alloys mainly exploited specific microstructural features, metastable phases, and refined eutectic phases that are produced during rapid solidification in AM samples.

It is important to note that, as of the date of this document's publication, the use of the ICME approach for certification of aircraft components is not consistent with a number of current FAA regulations that rely exclusively on test data (this is discussed in greater detail in Section 4). Nevertheless, leveraging ICME approaches in the product development process prior to the certification phase can still provide valuable insights and streamline testing efforts, contributing to more-efficient alloy design and optimization. Future advancements in regulations and modeling techniques may pave the way for broader acceptance of CM-driven approaches in the aviation industry, including both product development and certification.

3.4.4. Development & Acceptance of New AM Machine Architectures

The AM industry is experiencing an exciting phase of rapid technological advancement, and future machines are expected to incorporate novel capabilities, including dynamic process control driven by in-situ monitoring. However, these advancements pose challenges to conventional methodologies for material testing and qualification. To enable and harness the potential of these new technologies, CM and process modeling play a crucial role.

By employing CM approaches, industry can gain valuable insights into the process-microstructure relationships that occur during these advanced build processes. This information is essential for understanding how these new capabilities impact the final component's properties and performance. Additionally, CM allows us to analyze and bridge the gap between existing machine architectures and the new technologies being introduced into the AM industry.

As materials engineers and manufacturers embrace these advancements, model-based analysis becomes an indispensable tool for evaluating and optimizing the materials and processes within the context of the evolving AM machine architectures. This approach not only facilitates the successful integration of new capabilities but also provides a solid foundation for improving component design, performance, and overall efficiency in the future use of AM.

3.4.5. Accelerated *Delta Qualification* of Machines with Minor Hardware/Software Changes

AM equipment is continuously advancing, with numerous improvements, including increased build area size, multiple laser sources per machine, and frequent software upgrades. However, current part qualification standards mandate fixed machine states, materials, and process specifications. Any deviation from these fixed conditions necessitates an extensive re-qualification, known as delta qualification, which can take several months to complete. This lengthy and expensive re-qualification process hampers the rapid adoption of higher productivity additive equipment. It is especially impactful for parts where serial production may require many AM machines to achieve desired production rates.

The use of larger build volumes and multi-laser systems poses challenges due to the potential risks associated with increased process variation at the extremities of the build chamber and in regions where multiple lasers interact. To address these issues, a physics-based approach that predicts PSPP relationships virtually based on machine state and input process parameters can prove valuable. This predictive approach has the potential to reduce the time and expense required to re-establish optimal processing conditions and support materials testing.

By leveraging CM, along with in-process monitoring, engineers can virtually assess the impact of different machine states and process parameters on part quality and performance. This approach allows for efficient optimization of processing conditions without the need for extensive physical re-qualification. Moreover, it enables the exploration of novel machine configurations and process settings, fostering the rapid adoption of higher productivity AM equipment.

Implementing a physics-based modeling approach to virtually predict PSPP relationships holds significant promise in accelerating the adoption of advanced AM equipment and facilitating the exploration of innovative manufacturing processes. This approach empowers engineers to make informed decisions and effectively adapt to evolving machine capabilities, driving advancements in AM technology.

3.4.6. Quantified & Mitigated Build Variations

In the powder bed AM process, the structural and functional performance of fabricated components has been shown to exhibit variations from build to build (inter-build) and also based on the component's location and orientation within the build chamber, known as build chamber variation (intra-build) [28–31]. Understanding the causes and correlations of these variations with process parameters and input powder characteristics is crucial for Q&C of AM systems and components. The build chamber's varying conditions can lead to different microstructures and flaw populations, resulting from a multitude of process parameters, gas flow variations, heat source profiles, and powder spreading discrepancies. Input powder characteristics, for example, may change with powder source and powder reuse. Powder reuse practices may significantly affect both the economics and quality of a PBF-LB process for a given part, so use of validated CM models for assessment of the impact and limitations of powder reuse offers a structured approach for decisions and practices. This may be especially important for any parts with durability, fatigue, or damage tolerance requirements.

To comprehensively address this issue, computational materials tools for modeling the location specific build processes within real-world build environments are essential to quantify and mitigate build chamber variation. These tools can significantly reduce the time and resources required for testing during Q&C of aviation AM components. In the near-term, the focus will be on using computational materials tools to quantify the impact of build chamber variation on component performance. In the medium term, the objective is to pinpoint the causes of build chamber variation, identifying key process parameters and factors contributing to the observed variations. Looking further ahead, a long-term vision for computational materials tools is to effectively mitigate build chamber variation through a control loop that prescribes feature- or location-specific process parameters to the machine. This control loop will optimize the AM process based on the component's position within the build chamber, ensuring consistent and reliable performance across all parts. By integrating computational materials tools and implementing this control loop, the AM process can be fine-tuned to achieve consistent quality and enhanced performance for aviation components.

3.4.7. Implementation of Smarter Testing Inclusive of the Variation Across the Part

Since microstructures, properties, and operational conditions vary with location within the component, orientation of the part during the build process, and location within the build volume, traditional witness coupon testing is of limited value as it does not necessarily represent the AM-built component. CM engineering enables the user to develop representative test configurations. This ensures that the relevant variation in material properties is interrogated, potentially reducing the amount of characterization or testing required, as well as confirming the relevance of any test coupons to the part.

Addressing uncertainties in the AM process and impact on predicted property variations across different locations within the part requires development of a comprehensive model-based uncertainty analysis. A measurement test plan can be formulated based on the capabilities of measurement methods, part geometry, and statistical analysis results from the uncertainty analysis. Conducting a sensitivity study on the linked PSPP models can help rank each measurement location based on its influence on predicted properties. The required accuracy and precision of measurements for these specific locations can be determined, guiding the development of a measurement plan, including where to test and what test methods to use. This approach enables *smarter* testing, adopting zone-targeted testing, location-specific property assessments, and non-destructive methods.

Certification requires confirmation that any test coupons used are representative of the actual part being certified. CM engineering can enable development of coupons that are representative of the complexities of the actual part, providing a quantified approach to producing Process Equivalent Test Specimens (PETS).

By employing a CM engineering approach and implementing these model-based strategies, engineers can confidently optimize testing efforts, ensure the real-world relevance of test coupons, and enhance the certification process for AM components. This approach fosters a more-efficient and accurate assessment of part properties, contributing to the successful Q&C of aviation components.

3.4.8. Use of AM Build Process & Performance Modeling to Focus limited NDT Resources

Non-destructive methods are costly and time-consuming, especially when applied to larger, more complex, and structural or flight-critical components. Traditional methods may not be sufficient to detect relevant defects in these parts, leading to overly conservative requirements for their operational lifespan. However, the layer-by-layer nature of the PBF-LB process offers a unique opportunity for in-situ monitoring supported by modeling to localize, identify, and possibly correct defects during the build process. For example, by utilizing Physics-Informed Machine Learning (PIML) methods, thermal signatures combined with visible light imaging can produce localized quality metrics that are independent of part complexity, making them scalable to inspect large parts more effectively [32]. This or similar approaches, when coupled with materials performance models that consider in-service conditions, can explicitly identify regions of concern where additional attention is required. As a result, the burden on traditional NDT methods can be reduced by concentrating on these regions. This might be reinforced and to some extent validated by results of a commonly required quality demonstration: a detailed *First Article* inspection such as may be applied to forgings [33]. Here, a pre-production article would be subjected to extensive evaluation, including acceptance tests, dimensions, surface finishes, local microstructures, and NDE for defects. The *First Article* inspection may target risk areas of the component for more detailed review. Additionally, *First Article* assessment may also be required with a change in supplier, equipment, or process. Integration of CM modeling to address such a requirement could be very beneficial for Q&C efforts.

ML-based techniques have also shown the ability to improve the probability of detection for traditional NDT methods [34,35], further enhancing the inspection capability, especially in critical regions of a part. The localization of material quality and the improvement in inspection capability contribute to more accurate predictions of the part’s operational life, which, in turn, allows for a reduction in the required conservativism in lifing models.

By integrating in-situ monitoring, improved quality assessment, and advanced NDT techniques, engineers can gain a more comprehensive understanding of part quality and defect detection.

This integrated approach enhances the accuracy of part life prediction and allows for a more-efficient use of materials testing and inspection resources, ultimately leading to optimized designs and increased confidence in the performance of aviation components.

3.4.9. Enabled Rapid and Confident Decisions for Disposition of Manufacturing Non-Conformances in Production

With AM, as with any manufacturing process, there will likely be non-conformances in production. The implementation of validated analytical models for materials and processes offers the potential to rapidly and confidently evaluate manufacturing non-conformances. This would especially be true if appropriate in-process monitoring is employed. Decisions on whether to *accept as-is*, *reject* (i.e., scrap), or *rework/repair* could quickly be made and substantiated. For recurring non-conformances, the CM approach permits assessment of process modifications or improvements, especially within established process bounds, to reduce or eliminate future non-conformances. This represents the potential for significant improvement compared to the traditional *frozen process* approach, where extensive testing might be required to disposition non-conformances or approve process changes to prevent recurrences.

3.4.10. Q&C Decisions Based on Performance Risk Enabled by CM Engineering

The combination of simulation with UQ is a powerful tool in quantifying failure risk and uncertainty, especially in PIM technologies like AM. By leveraging computational models to simulate different scenarios, engineers can effectively identify potential failure modes and assess the probability of failure. A key component of this approach is the use of CM engineering tools. These simulations enable engineers to accurately predict material behavior and quantify uncertainty, providing valuable insights into material performance under various conditions.

Simulated, location-dependent, probability-of-failure maps are essential in this process, as they help engineers identify critical variables that significantly impact the safety and reliability of air vehicle systems. Informed by this information, engineers can prioritize testing and quality assurance efforts, and optimize experimental designs, leading to improved safety and reliability of structures while effectively minimizing testing timelines and costs.

Modeling-enabled failure probability predictions empower engineers and cost analysts to make informed engineering and business decisions, and enhance the overall performance and robustness of engineering applications, particularly in the context of PIM technologies such as AM. To realize these benefits, a higher degree of acceptance of these approaches by regulators is desired.

Section 4 Regulatory Considerations for CM Acceptance

4.1. Background

To enable a broader use of CM in the aviation industry, the regulatory considerations for Q&C of materials and components manufactured using PIMs, including AM, need to be identified and addressed. The intent of this section is not to define a comprehensive list of such considerations or regulatory acceptance criteria, but rather to provide a high-level overview of relevant regulatory enablers and key drivers in the context of this CM4QC document, as well as potential future actions. Further discussions and comprehensive engagement of the CM community of practice with the regulators, both commercial and military, is needed to identify specific acceptance criteria for CM models, current regulatory gaps and the paths to address them, guidance for CM models application in the context of certification projects, etc.

4.2. Current State

Historically, there has been a heavy emphasis on the use of test data in characterizing performance of materials at different scales of the test pyramid (see the notional test pyramid in Figure 4.1), which is reflected in many of the current aviation regulations and supporting guidance materials. Such emphasis was influenced by the lack of predictive CM capabilities over the past few decades that gave rise to empirical approaches, and the overall positive field experience and safety record with using such testing-based methods. At the same time, the regulations, airworthiness standards and guidelines of several agencies (e.g., United States Air Force (USAF), Naval Air Systems Command (NAVAIR), and NASA) are largely neutral to the use of CM, and do not explicitly restrict its use in the context of certification projects. For instance, the latest NASA AM Standard [2], remains neutral on the topic of CM use.

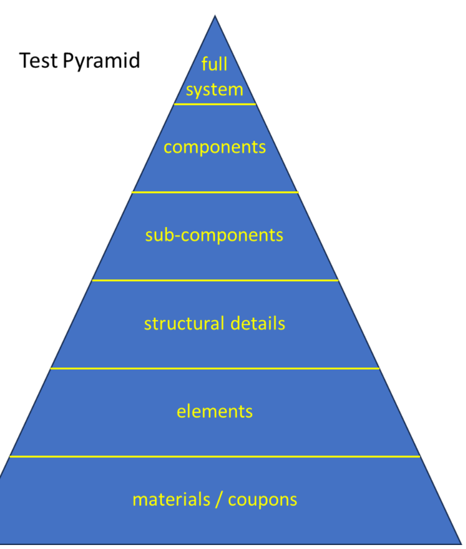


Figure 4.1 Notional aviation test pyramid

The level of acceptance of modeling and simulation in general, and CM in particular, varies across the FAA regulatory domains and product types. For instance, the rules addressing material or manufacturing requirements (e.g., [36–38]) for airframe structures only allow the use of test data. At the same time, fatigue and damage tolerance (F&DT) regulations (e.g., [6,39]) and a number of other areas allow the use of "analysis supported by test evidence" or "validated analysis." However, the specific requirements for this approach (e.g., what level of supporting test evidence is required) are typically not spelled out, and the detailed implementation is left up to the applicant working in close coordination with the appropriate FAA certification office. Finally, only in a limited number of examples and applications is the use of modeling explicitly permitted as an alternative to test-based methods (e.g., [40]), albeit subject to specific restrictions and limitations.

The current state of DOD regulatory or customer requirements with regard to DOD systems is somewhat similar. There are overarching specifications for aircraft and propulsion systems [4,5,41,42], but these do not call out specific requirements or discuss acceptable methods of compliance. The most detailed requirements are found in MIL-HDBK-1783B "Engine Structural Integrity Program (ENSIP)"[43] and MIL-HDBK-1587, "Materials and Process Requirements for Air Force Weapons Systems" [44]. However, unlike the commercial aircraft and engine regulatory requirements, the specifics of contractual requirements are negotiated between the applicant (the program managing entity) and the corresponding DOD agency. These DOD standards are pointed out here because the approaches for achieving industry-wide CM- and model-enabled Q&C for PIM must consider both DOD and commercial aviation applications. Regardless of the application domain, comprehensive – and persuasive – VVUQ would be essential for successful implementation.

It should be noted that, while many practitioners consider the outcome of the test pyramid -based approach to represent the *ground truth*, there are some known limitations of this approach, including the lack of physics-based understanding of the connectivity between the different layers of the test pyramid, lack of predictive capabilities (that could help minimize programmatic risks), as well as a number of considerations discussed in Section 4.4.

4.3. Regulatory Enablers

As discussed elsewhere in this document, development and maturation of the CM frameworks and their effective use in aviation applications requires a considerable level of investment. In order to capitalize on such investments, the companies need to advance their product to the highest TRL, including the certification phase and field deployment. This, in turn, requires a high degree of organizational confidence in the CM predictive capabilities. Gaining such confidence, and therefore a higher level of regulatory acceptance, can be achieved through a consistent and rigorous application of a number of methods and frameworks, including the implementation of CAFs, conducting V&V and UQ of the models, TRL/SML assessment, etc. A set of guidelines and acceptance criteria will need to be developed through a close collaboration between the regulators, end-user community (e.g., OEMs, DOD), and methods developers. To be effective and practical, the methods and criteria would need to be scalable and will depend on the criticality of application, the extent to which CM is used in the certification process, and other relevant considerations.

In addition, it may be beneficial to *extend* some common regulatory practices to CM-informed Q&C for PIMs. As an example, damage tolerance assessments are required for critical locations of many parts in DOD aerospace applications, and for some high-risk components for commercial aerospace applications [39,43,44]. Consider that for PIM, use of CM models could enable identification of high risk (or high-uncertainty) part locations for specific applications, consistent with the part zoning approach discussed in [45]. Once identified, such locations could be subjected to damage tolerance assessment requirements to serve as a risk mitigation step and to provide additional confidence for acceptance of CM-enabled Q&C practices. This approach could be defined in the context of the relative criticality of the specific material, process, and application.

4.4. Additional Drivers for Increased Regulatory Acceptance of CM

While the gradual reduction in conventional Q&C test matrices is commonly cited as a key benefit of the greater acceptance of CM methods by the regulators, this is by far not the only area where the broader use of CM can add value. Additional potential benefits from the perspective of the regulatory agencies include:

- Enabling (through the use of CM and UQ) the use of quantifiable risk-based metrics for material and part performance assessment and qualification
- Optimization of material test matrices informed by CM insights (i.e., getting the most valuable information out of the fixed level of testing)
- Exploring the corners and fringes of the multi-dimensional process parameters space (that would be impractical to explore using conventional test methods) in order to fully capture material performance variations and to better understand 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 versus actual parts
- Addressing the known shortcomings of a test-based approach, as discussed at the end of Section 4.2

It should be noted that the concept described in the second bullet above is not new, nor is it unique to aviation applications. For instance, according to Ref. [46], the Food and Drug Administration (FDA) has accepted model-based approaches (*in silico*) as possible replacement for animal testing to explore rarely-occurring manifestations of the phenomena in question during pre-clinical assessment. This methodology is part of an overall risk reduction approach that enables “the detection of unexpected severe adverse events too rare to be detected in a clinical trial, but still likely enough to be of concern.”

When comparing conventional test-only Q&C methods with the use of CM model predictions combined with testing, it should be noted that even the methods based exclusively on testing are not devoid of risk; test data always has a certain level of experimental error, and the specific testing setup represents an approximation of physical reality that also has an uncertainty or error associated with it. These considerations should be factored in when comparing the merits and risks of the conventional test-only frameworks with CM-enabled methodologies, including potential CM benefits for systemic risk reduction outlined above.

CM frameworks, once properly developed and validated, could offer unique physics-based insights into the PSPP relationships that cannot be achieved with the use of test-only methods. For instance, going forward, CM combined with the appropriate level of supporting test evidence may be the only viable option for certification of PIM in some specialized aviation applications.

4.5. Balance Between Test Data & CM

The goal of increased use of CM in the Q&C of PIM in aviation applications is not to *replace* testing, but to enable *smarter testing* [22,47] and to find an optimal balance between the testing and modeling as notionally shown in Figure 4.2.

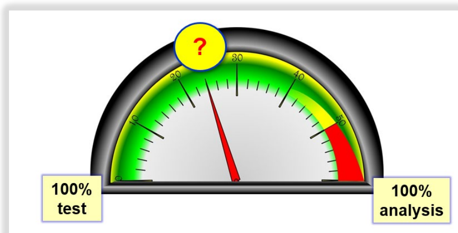


Figure 4.2 Notional graphic showing a balance between test and analysis

Furthermore, as the use of CM gradually increases, there will be an inevitable redistribution of testing resources whereby a significant subset of test data would need to be used for model development, calibration, V&V, and UQ. Some of these resources therefore would be used to increase the understanding of the underlying physics, as opposed to the currently dominant fully empirical frameworks.

4.6. Future Work

A broader regulatory acceptance of CM is required to fully realize its benefits in the Q&C of aviation products. To achieve this state, the following implementation elements are recommended:

- Identification of the regulatory gaps impeding the broader use of CM, and development of a plan to address these gaps
- Development of the regulatory guidelines and/or public standards for the acceptable levels of VVUQ for CM models, commensurate with the application's criticality, SML, and the extent of CM utilization
- Development of the methodologies and guidelines for the generation of *hybrid* allowables where conventional test data is supplemented by CM predictions
- Development of the CAF considerations for the use of CM models and simulations, especially in high-criticality applications (e.g., via public standards)
    - Note that the CAF standard for Airframe Structures Modeling & Simulation is being developed by the ASME VVUQ-90 sub-committee, and many of its elements are expected to be applicable to CM.

- Development of methodologies and guidelines for integration of CM models and simulations with Quality Assurance methods during manufacturing (e.g., in-process monitoring and control)
- Development of illustrative examples of CM application, V&V, and UQ that could be used for training and education of the regulators and applicants
- A close collaboration between the regulators, industry, and SDO’s in addressing the above areas

Section 5 Key Computational Materials Capabilities & Enabling Technologies

5.1. Introduction

This section focuses on CM tools that can predict relationships, with quantified uncertainties, for PSPP of metal additive parts. The complicated scan paths, extreme thermal histories, and rapid solidification in AM can lead to microstructures (including grain morphologies, secondary phases, solidification microstructures, flaws, and surface roughness) that are often distinct from those of other more established manufacturing techniques. These microstructural differences, often exacerbated by non-optimized post-build annealing treatments, in turn affect the material properties and ultimately the performance of parts. CM tools have been developed to predict these PSPP relationships throughout the relevant range of length and time scales, ranging from the macroscopic part scale to micro- and even nano-scale structures; a number of these tools are discussed in some detail in Section 5.2. The specific topic areas are 5.2.1) Process Modeling and Simulation, 5.2.2) Microstructure Modeling and Simulation, and 5.2.3) Property and Performance Modeling and Simulation. In addition to CM simulation tools themselves, additional technologies and activities are needed to improve the accuracy and efficiency of validated models and to reduce variability and give repeatable and predictable performance across multiple AM machines. These enabling technologies and needs are reviewed in Section 5.3. The specific topic areas for this section are 5.3.1 Measurements, 5.3.2 Multi-scale and Multi-physics, 5.3.3 Machine Learning and High-Performance Computing, 5.3.4 Digital Twins and CM4QC, and 5.3.5 Standards.

5.2. Key Computational Materials Tools

The goal in using CM methods for AM processes and parts is to establish the quantitative relationship between processing conditions and all relevant structural (and functional) properties of the material, as well as the performance of the part under specified applied loads and environmental conditions. The material properties and performance are the result of the microstructure in combination with the flaws present in the material, which themselves strongly depend on the thermal history of the material during and after solidification. Figure 5.1 illustrates a simplified framework for PSPP modeling, in which thermal and melt pool dynamics modeling of the AM process inform the prediction of microstructures and flaws; these in turn can be used in models over multiple scales to predict material properties and part performance.

Figure 5.1 PSPP modeling framework, showing a simplified subset of computational paradigms. Models at both the part-scale and the melt pool-scale are necessary to capture the complex thermal history and flow dynamics of the material, which in turn drive the formation of microstructure and flaws such as porosity. An understanding of these microstructures and flaws allows the prediction of material properties and part performance under a given load or usage environment. Modeled phenomena span scales from the part scale (cm or m) down to the micrometer or even nanometer scales. Accurate modeling with quantified uncertainty may allow process and design optimization, improved process control, and reduced testing for qualification of parts. Subfigures taken from references [48–52].

In the remainder of this section, the individual models and capabilities that comprise this framework are described.

5.2.1. Process Modeling and Simulation

Thermal modeling: part scale

Because the temperature field and its variation in space and time affect all aspects of the material structure, any modeling pathway must begin with a prediction (or approximation) of the thermal history. This multiscale problem includes length scales spanning from the laser spot size and melt pool dimension (≈ 100 μm) to the part size (10 cm or larger), and time scales ranging from sub-μs to days. Thus, simulation of the entire detailed thermal field in space and time is infeasible because of computational expense and data storage limitations. Approximations are therefore typical when simulating at the part scale. For example, models may ignore fluid flow in the melt pool [53,54], rely on reduced-order or data-driven surrogate models to capture the interaction of the melt pool scale with the complex geometry of the part itself [55], or leverage a limited set of strategically selected high-fidelity models to inform a lower-complexity model to achieve the desired computational efficiency (see later discussion in 5.3.2). When predicting distortion or residual stress, the thermal strain of entire layers or groups of layers (*lumped layers* or *superlayers*) at a time may be approximated together to allow the efficient calculation of displacements over the entire part [49,56]. However, because the scan pattern can strongly affect residual stresses [57], these lumped layer approaches may not be effective for simulating residual stress distributions. Intermediate beam agglomeration approaches using a scan pattern with enlarged melt pools can more accurately model these stresses [57]. Furthermore, calibration of the parameters of approximate models such as superlayers remains a challenge as some of the model parameters may not be directly observable using experimental measurements.

Thermal modeling: track scale

Approximations like superlayers are not as useful when predicting other microstructural aspects, like grain structure and solid-state phase transformation products, because the metal microstructure is sensitive to details of the thermal field such as temperature gradient and cooling rate at the length and time scales of the melt pool. Simulations that capture the necessary level of detail are typically limited to individual or small numbers of laser tracks and build layers, usually at or below the millimeter scale. Heat flow can be simulated at the scale of the individual melt track using standard commercial FEA tools. One direct application is the prediction of melt pool size and shape, which feeds into the prediction of, e.g., lack-of-fusion (LOF) porosity (combined with hatch spacing and layer thickness).

Calibration is required because of boundary conditions, mainly those associated with the heat source, such as surface absorptivity, but also to some extent those that describe heat loss, such as surface convection coefficient. Even in conduction mode, for which molten fluid motion and surface deformation are small, the effective absorptivity varies widely among different materials which makes this a first-order calibration requirement.

Another complication is that effective absorption is not actually constant and can vary substantially even for nominally uniform processing conditions, especially near the keyholing transition regime. Melt pool-scale models that neglect complex fluid flow and free-surface deformation mostly assume constant effective absorption. This approach also does not capture stochastic variability in melt pool dynamics. The literature reports a wide range of calibrated effective absorptivity values in FEA models even for the same material processed by the same parameter set [58,59]. This variation is mainly due to the neglect of some heat loss mechanisms (e.g., surface convection, radiation, evaporation, phase change) to gain higher computational efficiency, resulting in a calibrated absorptivity that is smaller than the measured value. In addition, there is the issue of the shape of the heat source on the metal surface, e.g., ring versus top-hat versus Gaussian. For heat loss, attention must be paid to the details of the scan pattern and the local part geometry, for example, whether a thin wall or overhang is being printed. Current efforts to apply UQ to simulating melt pool dimensions are mostly confined to basic quantities such as depth and width, for example, [60].

Validation data from single tracks is available via numerous publications that provide cross-sections of melt pools along with process parameter values such as power and scan speed; AM Bench provides easily accessible examples of this sort of data along with in-situ measurements of melt pool length [61,62]. Notwithstanding current efforts in benchmarking, developing a dataset for full UQ on melt pool dimensions and shape remains a significant challenge and may require, for example, a combination of top-down videography and/or absorptivity with side-view x-ray radiography [63–66].

Thermal modeling: melt pool flow simulations

Even if the FEA thermal model can accurately simulate the measured width, depth, and length of the melt pool, it may not accurately predict the cooling rate as the temperature distribution inside the melt pool does not usually match well with Computational Fluid Dynamics (CFD) simulations, especially in the mixed conduction/convection and keyhole regime [67]. Fluid flow predictions in the melt pool can also shed light on phenomena like porosity, surface roughness, and spatter. Melt pool-scale modeling is a CM tool that can help an engineer establish reliable operation of a 3D printer, especially if they would be starting with a completely new printer and aim to predict printing outcomes starting with only basic information about the machine. There is, for example, substantial evidence that significant interactions occur between the power source (laser light or electron beam), the metal (solid, liquid, or powder), the flowing cover gas, and the vapor plume [68–70]. Fluid flow in the melt pool under laser (or electron beam) illumination is complex and sensitive to all these factors and interactions. It is particularly important to include the details of the laser light since, for example, the spot size (and shape) influences the power density, which in turn influences the occurrence of metal boiling and the stability of any resulting keyhole. It also affects the net absorptivity, which is a first-order influence on melt pool dimensions and shape [71,72].

One example of potential use of fluid flow modeling is the prediction of the humping, under-cut, and balling-up phenomena because there appear to be practical limits to how much one can increase power and speed to increase productivity [73]. Theoretical models seem inadequate so direct numerical simulation can contribute; multi-fidelity models that combine both types of models have also been studied [74]. Another example is the prediction LOF porosity, which as previously mentioned is due to incomplete melt pool overlap. Most models assume a constant melt pool geometry (width and depth). In reality, however, melt pools exhibit variability [75], so fluid flow simulation could help to predict and account for this variability. Similarly, the instability of fluid flow gives rise to so-called spatter particles, i.e., droplets of liquid metal and partially melted powder ejected from the melt pool [76].

Melt pool-scale models that capture the laser-powder interactions, solid-liquid (and even vapor and plasma) phase changes, and melt pool flow with moving interfaces are available in both commercial software and research codes [77–79]. Some of these codes use traditional continuum solutions of the Navier-Stokes equations, volume-of-fluid [80] or level-set [81,82] techniques to model the moving interface; others use the lattice-Boltzmann method [83,84] to simulate the multiphase flow field.

Data are available for validation of melt pool flow simulations from high-speed videography and from high-speed x-ray radiography. Even radiography with synchrotron radiation X-rays provides only a 2D projection and marker particles are needed to visualize fluid flow. Trends can be compared between experiments and simulations; however, full validation in 3D is computationally intractable for all practical purposes.

Finally, we note that gas flow in the chamber of a PBF-LB printer is known to be important to minimizing flaws through its main functions of decreasing laser/plume interactions which have been seen to decrease local melt pool depth by more than 30% [61,85], and carrying condensate, ejected particles and spatter particles away to prevent flaw formation via re-deposited particulates. Simulations of gas flow [86] may be used to address these issues, and support design of inlet grids, nozzles, and other components as a part of AM machine development.

Residual stress and distortion prediction:
The high temperature gradients and rates of change characteristic of AM lead to thermal-induced residual stress in manufactured parts that cause distortion and sometimes cracking of the as-built parts; these can lead to recoater blade crashes and build failures. The dominant reason for the occurrence of residual stress in AM is the same as it is for welding in that relaxation of the high temperature gradients that are present following solidification of the melt pool produces differential thermal contractions that are only partially relaxed through plastic deformation. Pre-heat is thus the most effective mitigation for residual stress (and cracking). The amount of residual stress present also affects part performance such as fatigue and creep, and large residual stress may lead to solid-state cracking if it exceeds the material strength.

Modeling of this stress and distortion allows for compensation of the prebuild geometry of the part such that it distorts to the desired part geometry or for mitigation/minimization of the distortion through optimal design of the part or process. Residual stress/distortion is often most efficiently approximated using the inherent strain method [49,56,87], either by assuming a constant eigenstrain that is usually determined from experimental data, or using a calculated eigenstrain with an assumed temperature difference between the solidification temperature of the material and the underlying substrate. To make the residual stress calculation tractable, the simulation is typically done not at the individual laser track scale, but by adding entire layers or groups of layers (superlayers) at a time.

Evidence for recent success in predicting residual stress is found in the 2022 round of AM Bench [88] (see Appendix V, Figure A2.1) in which the first place prize for the “Residual Elastic Strains” challenge was won by an AM software solutions company. Although this suggests that the leading software tools have matured and are usable in an industrial setting, analyst skill remains essential mainly for correct application of boundary conditions. The successful matching of simulations to experimental data (i.e., validation) in public challenges such as AM Bench also provides evidence of validation data becoming available. Even where commercial vendors make validation data available, it is rare that users’ needs correspond to the bounds on the variables in the data provided. Each user, in general, is responsible for their own validation (see Section 6).

While models and commercial codes are matured for predicting macroscale (Type I) residual stress, there is little work on predicting the location and time that solid-state cracking occurs during the process, as well as modeling microscale (Type II) residual stress, which is critical to understanding solidification and liquation cracking and fatigue.

Porosity and Flaw Prediction:
Porosity is the most prevalent flaw in AM, particularly in PBF-LB and binder jet printing, and can be caused by multiple phenomena. LOF porosity is caused by insufficient overlapping of melt pool tracks, leaving unmelted volumes characterized by irregular, non-spherical pores between powder particles. Most LOF porosity can be avoided through proper selection of process

parameters to ensure fully overlapping melt pool tracks [89]. However, local variability in the melt pool size may still lead to unexpected LOF porosity. This variability may be due to effects of feature geometry on the local heat transfer, reheating from complex laser tool paths, the stochastic nature of the powder geometry, flow instabilities in the melt pool, interaction of the laser with the vapor plume, etc. Irregularities in the melt pool shape lead to stochasticity that should be accounted for when predicting melt pool overlap and mitigating LOF porosity.

Another common type of porosity is keyhole porosity. The keyhole is a deep depression of the fluid-vapor interface at the melt pool surface caused by evaporation recoil forces. Flow instabilities may lead to collapse and breakup of the keyhole, resulting in gas bubbles that, if overtaken by the solidification interface before reconnecting with the surface, remain as pores (typically more spherical in shape than LOF pores) in the resulting part [90]. Related to this is spatter formation which has been shown to be related to process conditions adjacent to unstable keyholes [91]. Detailed physics simulation of the formation of keyhole pores requires CFD models at the melt pool scale that can accurately capture the keyhole formation and breakup, including the complex interaction between the laser and the moving molten interface [92]. Such models are available in some commercial CFD codes, but they must be carefully calibrated and validated and are subject to large parameter uncertainties (e.g., those controlling the laser absorption and the surface tension gradient). Such simulations have been more successful in providing scientific insights into pore formation mechanisms than in providing quantitative predictions of porosity. Other approaches to predicting porosity, including data-driven models based on process input parameters or in-situ melt pool measurements, have shown recent promise [63].

Porosity may also be caused by gas that is entrapped in the feedstock powder (which is difficult to predict with computational materials tools) [93], or by interdendritic cavitation due to density changes during solidification [94]. This latter form of porosity is closely related to hot cracking seen in AM and other solidification processes and may be treated with similar modeling approaches. Another type of porosity can arise from the entrapment of gases in-between the powder particles that rise toward the surface but are unable to escape before the melt pool solidifies.

Surface roughness prediction:
AM-built parts are often characterized by surface roughness at the layer- or powder-scale. This roughness varies depending on surface angle, scanning pattern, and gas flow direction and may even be sensitive to subtle details such as powder spreading parameters. While roughness can be mitigated by post-treatment, such treatment may be difficult for complex geometries or internal features – exactly the features of a part that may make AM an attractive choice for production. In principle, surface roughness might be predicted by simulating the build of a large number of layers using melting and powder spreading models, which is a numerically intensive effort. However, because of the range of length scales involved, very little progress has been made toward directly simulating the formation of surface roughness; its prediction may require data-driven empirical approaches including ML models [95]. An additional complication that is important to address is related to the surface roughness measurement itself, which is dependent on the measurement technique (most rely on line-of-sight to the surface features of

interest, which is not always a complete picture), the size of the measuring instrument, and the length scale being measured. It is also important to realize that surface-initiated fatigue cracks initiate from stress concentrations at valleys whereas the most obvious feature of as-printed surfaces are the unmelted particles [96].

Powder flow modeling and simulation:
Powder spreading is generally simulated with the discrete element method (DEM), for which both open-source and commercial software programs are available. DEM is capable of modeling with a range of powder sizes although non-ellipsoidal particle shapes are significantly more expensive to simulate [97]. For example, DEM can predict areas that are low density (of packed powder) in the vicinity of sharp edges in the height of the part; after a few layers accumulate, the low density patches are likely to lead to porosity with the appearance of LOF [98]. For powders with strongly non-spherical shape, powder flow simulation can predict the variability of powder packing density with similar results in terms of LOF porosity. For process modeling that includes on-the-fly prediction of distortion correction, simulating powder flow (in principle at least) allows mitigation of gaps, denuded zones, and streaking in powder spreading (and, in turn, porosity). Examples of use in practice include work performed under the Defense Advanced Research Projects Agency (DARPA) Open Manufacturing Program [99]. Nevertheless, what remains lacking is a quantitative connection between the available measurables for powders and their *printability*.

5.2.2. Microstructure Modeling and Simulation

The prediction of material microstructure, including microstructural flaws that can lead to premature part failure, is a challenging problem because of the complex phenomena and multiple length and time scales involved. Commercial tools for predicting microstructure, including grain structure and flaw formation, are uncommon and for many applications are non-existent. Flaws of different types may develop during the build process and during post-build processing. Flaws, defined broadly, encompass deviations from the designed geometry and material. They include microstructural flaws like microcracks and undesired solid phases or heterogeneities, as well as morphological flaws such as pores, cavities, and surface roughness. These phenomena are often deterministic at the macro-scale, or when viewed on a statistical basis, even though they may be locally stochastic in nature (e.g., a fluctuation in powder packing density) and occur at length scales inaccessible by part-scale or even many melt pool-scale modeling approaches. Effective predictive approaches, therefore, are expected to be a combination of high-fidelity simulation models that can capture these small scales (from the atomic scale to the melt pool or powder scale), along with more-efficient computations at larger scales that rely on empirical models that are calibrated and validated with measurement data for the material and geometry of interest. Both types of models are likely to possess large uncertainties caused by both lack of knowledge of material and process parameters and the inherent stochasticity in the formation of flaws. Post-processing, such as heat and pressure treatment, further modifies the microstructure and flaw state and must be modeled; understanding the as-built state of the material provides an important initial condition for post-build processing simulation.

Computational thermodynamics and thermo-kinetics:
CALPHAD is a well-established technology for which commercial and open-source software tools are available. The prediction of equilibrium phases for alloy systems at a given composition and temperature can be done very accurately, as long as databases are available with the sufficiently accurate phase-based property data, such as the Gibbs energy, for a given system [100]. More difficult are thermo-kinetic calculations needed to describe the time evolution of material that is not at equilibrium, which is especially important given the fast solidification rates of AM; for example, metastable phases that appear due to non-equilibrium and rapid solidification in AM are not necessarily included in material databases [25–27]. Microsegregation at the dendrite scale can lead to large local variations in composition, which in turn affect phase changes and precipitation during manufacture and subsequent heat treatment [101]. Models of these phenomena typically rely on simplifying assumptions and require a large number of uncertain parameters, such as diffusion coefficients, interfacial energies, and nucleation site types and densities. These microstructural features also change in non-equilibrium conditions and need further calibration for AM samples. Furthermore, in contrast to equilibrium simulations, the thermo-kinetic calculations are very time-consuming and will benefit from acceleration via reduced-order models or in combination with machine learning techniques [25–27].

Several commercial packages for CALPHAD are available and widely used. It is generally understood that the predictions of phase relationships, for example as graphed by phase diagrams, are as reliable as the underlying experimental data. These data are used to calibrate thermodynamic functions that quantify the Gibbs free energy of each phase that might appear for a specified set of component elements. Thus, the reliability of the predictions is directly related to the availability of these functions for whichever alloy system (i.e., specific combinations of elements) is of interest. These functions depend on the availability of properly evaluated experimental data with more recent inclusion of first-principles calculations of energies of formation of compounds (at zero temperature); the latter are often at least as reliable as experimental values, although the computational expense can be very high. Although a body of literature on UQ in CALPHAD exists, such tools are not yet available in commercially supported packages. As an example of state of the art of UQ, confidence bands can be computed for phase diagrams: see, for example, Ref. [102]. Extensions of CALPHAD methods to include kinetics are also widely available and rely on availability of experimental diffusion databases.

Grain-scale microstructure:
Several classes of methods have been developed for the prediction of as-built grain structure in an AM-built material at the melt pool scale. Common assumptions include no nucleation of new orientations and epitaxial re-growth of solid from the heat-affected zone (HAZ). One may further assume that growth along <100> directions is strongly favored in cubic metals (including most commercially available structural alloys) with the overall growth direction determined by the temperature gradient. The most prevalent techniques are geometric approaches [103], grain-scale phase field (PF) [104,105], cellular automata (CA) [106,107], and kinetic Monte Carlo (KMC, also known as the Potts model) [108,109]. The main input to all these methods is the

temperature history during solidification, most often from a thermal or CFD simulation but occasionally from analytical or semi-analytical approximations.

Grain-scale PF models solve a partial differential equation (PDE) for a set of order parameters that identify individual grains. The PF formulation captures the evolution of the free energy of the system, including anisotropic interfacial energy. PF simulations are typically the most computationally intensive of the three approaches discussed here. CA methods rely on a set of rules for grain evolution, rather than a well-defined set of equations, and use subgrid models for grain nucleation and dendritic growth velocity to predict the progression of a developing microstructure. CA is less computationally demanding than PF models and has been used to predict AM microstructure on domain sizes comprising multiple laser tracks over hundreds of layers of growth to achieve millimeter-scale predictions [110]. The KMC method is also lower in computational expense compared with PF. In KMC, lattice sites may randomly change their grain association such that the total energy (usually the interfacial energy) decreases with time, mimicking a growing grain structure.

Commercial implementations are not yet widely available for any of these three approaches, although first prize for the microstructure challenge problem from AM Bench 2022 was jointly shared between two competing groups, one of which was an AM software solutions company. Nevertheless, most of the recent development and demonstration of microstructure prediction has been done by government or academic researchers; some open-source code is available (e.g., the Stochastic Parallel PARticle Kinetic Simulator (SPPARKS) code for KMC supported by Sandia). Data are available for validation of such simulation tools, e.g., from the first and second rounds of AM Bench [111,112]. A related needed technology for validation is the ability to quantitatively describe and distinguish complex microstructures; since grain size alone is not sufficient to characterize AM microstructures, statistical descriptions such as crystallographic orientation (texture), higher-order correlation functions [113] and ML approaches similar to those used for image recognition [113,114] are being explored for this problem.

Sub-grain microstructure:
Micro-segregation occurs in many metal alloys even under the rapid solidification conditions of metal AM. This phenomenon can be readily modeled with commercial CALPHAD tools using the Scheil model (and modifications thereof), albeit limited to one dimension [115]. More detailed physics simulation at the dendrite scale is usually achieved through PF models, formulated slightly differently from the grain-scale PF models described previously in sub-section *grain-scale microstructure*, to solve for order parameters and composition variables during dendrite solidification [116]. Formulation and solution of such models for real alloys is a challenging problem and closely linked to the availability of thermodynamic information, along with validation against experiments. Data-driven approaches may be possible, since dendrite spacing and other sub-grain microstructure statistics can be correlated to thermal history variables such as cooling rate [117].

Another aspect of sub-grain microstructure that is important in predicting material properties and part performance is the formation of precipitates, both during the build process itself and during subsequent heat treatment. Again, development of well-validated PF simulation is a possible approach to obtain detailed prediction of precipitate formation [118]. Thermo-kinetic models that predict precipitates in a more statistical sense, such as volume fractions, are available [119]. As described previously in *Computational thermodynamics and thermo-kinetics*, these thermo-kinetic models require specification of a large number of parameters, many of which may not be known with adequate precision. Additionally, precipitation modeling requires an accurate knowledge of the initial composition of the material, which for AM-built material may fluctuate substantially locally from the expected composition because of micro-segregation during the rapid solidification process [101] and macroscopically due to vaporization of volatile alloy elements or inclusion of environmental contaminants (e.g., oxygen).

Microsegregation, precipitation, phase transformation, recrystallization, and grain growth may also develop during secondary processing, for example, part removal from the plate, stress-relief, hot isostatic pressing (HIP), machining, shot peening, chemical etching, forging, homogenization, and annealing treatments. Such processes of microstructural evolution are also amenable to simulation. However, the various simulation tools have varying levels of maturity which are not assessed here; see Section 9 for further details.

In-process cracking: Solidification cracking, or hot cracking, is a well-known phenomenon in casting and welding processes that can be worsened in AM because of the large temperature variations and resultant thermal stresses, as well as the anisotropic microstructures common in AM [94,120]. Hot cracking most often occurs in the late stages of solidification, near the solidus temperature, and is caused by an insufficient flow of molten metal to balance the solidification shrinkage in the inter-dendritic spaces. In-process cracking thus depends on the material behavior near solidification, the details of the spatially and temporally varying temperature field, and the morphology and flow permeability of the microstructure. Detailed computational simulations of these phenomena are not available, and so prediction and mitigation of solidification cracking typically relies on phenomenological models and empiricism, albeit informed by CALPHAD modeling [121–123]. Other cracking mechanisms such as solid-state cracking (e.g., cold cracking, or ductility dip cracking) as well as high temperature properties (e.g., ductile-to-brittle transition temperature, elasticity) are also important.

5.2.3. Property & Performance Modeling and Simulation

Microstructure-to-properties modeling and simulation:
The relationship between microstructure and material mechanical properties has long been a research topic for traditionally manufactured materials. Phenomenological models exist relating aspects such as grain size and precipitates to strength and fatigue life [124]. For example, the well-known Hall-Petch equation relates grain size to yield strength (YS) and involves material-dependent parameters that must be obtained experimentally. Similarly, the effects of precipitates and other subgrain microstructural features on material properties usually must be quantified experimentally. First principles calculations are also possible: the tensorial elastic modulus as a single crystal property is calculable, as is temperature dependence albeit at greater expense.

The detailed multiscale simulation of the effects of complex microstructures on macroscale properties is a research topic that continues to become increasingly important. Furthermore, the AM process results in microstructures that are markedly different from other processes, including anisotropic grain structures and textures and characteristic flaws such as LOF pores. The anisotropic elastic modulus of a polycrystalline material is readily computed to first order from a knowledge of the single crystal properties and a list of orientations with volume fractions (texture). YS is extremely sensitive to microstructure, composition [125], strain rate, and temperature [126] because it depends on the population of obstacles to dislocation motion [127]. Commercial tools to predict YS depend on a knowledge of the thermodynamics of the system combined with a knowledge of the nucleation density, precipitation kinetics, and a detailed thermal history of the material.

Existing tools typically focus on near-spherical precipitates even though the actual phase morphology can be more complex as in, e.g., lamellar structures found in steels and Ti alloys. Multiple examples exist in the literature of successful use of these tools. It is also important to note that prediction of mechanical behavior is not limited to YS but also includes plastic behavior as a function of temperature and strain rate, etc. Where the crystal/grain orientations are non-random, i.e., texture is present, anisotropy is then a function of that texture as well as the grain shape, which in turn means that relative values of critical resolved shear stresses must be determined [128]. These data provide the basis for crystal plasticity simulation, see next sub-section.

Creep and fatigue:
Performance of additively manufactured materials under fatigue and creep loading is highly dependent on localization phenomena, resulting from surface roughness, microstructural heterogeneities and flaws. The current state of engineering practice does not adequately consider these phenomena. Rather, it is exemplified by commercial software tools that implicitly account for microstructure and flaws via calibration to continuum-scale coupon test data but do not consider microstructure and flaws in a physics-based manner [129,130].

Crystal plasticity (CP) simulations have been developed for prediction of local deformation (e.g., plastic slip accumulation) that results from dominant material characteristics, loading conditions, and environmental factors, and are readily coupled with explicit damage modeling and multiscale modeling approaches. CP simulations have also provided valuable insights regarding the plastic slip accumulation at the boundaries of contiguous hard and soft grains that have been identified as crack initiation sites during creep/dwell-fatigue scenarios. A significant challenge in creep modeling is the choice of the constitutive relation(s) to be used. Although there is a substantial literature on the general issue of modeling and simulation for creep, AM leads to novel microstructures that may require new parameterizations to existing models or new model development [131].

Within the context of fatigue, once the state of local deformation is determined from the output of CP simulations, fatigue indicator parameters can be employed to estimate the number of cycles to fatigue crack nucleation. These indicators typically quantify accumulated plastic strain or energy metrics that correlate with experimental observations of crack nucleation. Beyond fatigue indicator parameter-based approaches, crack nucleation and propagation models incorporating damage parameter evolution or explicit crack geometry representations are increasingly used to precisely characterize local material failure mechanisms. These approaches enhance the base CP models by incorporating progressive degradation of material properties and explicit representation of discontinuities that develop during cyclic loading.

When integrated with developing capabilities for process-structure simulation and uncertainty quantification, these structure-property/performance simulation capabilities will form the foundation for an envisioned computational materials-informed ecosystem for predicting fatigue and creep behavior of PIM through integrated multi-scale, multi-physics simulation, characterization and monitoring.

5.3. Key Supporting Technology Needs

5.3.1. Measurements

Measurement of parameters for calibration and validation:
Among the inputs needed for the computational models discussed in Section 5.2, material properties likely include the largest uncertainties. While some important thermophysical properties such as density and thermal conductivity are known for most materials of interest, the extreme thermal excursions characteristic of AM processes require knowledge of the temperature dependence of these properties far from the normal operating range, including in the liquid phase. Thermophysical properties such as viscosity and surface tension of molten metal are not usually well characterized, especially as functions of temperature or composition; others, such as surface absorptivity, may be highly variable depending on the environment.

As an example, surface tension is a key thermophysical property that is strongly sensitive to surface segregation, as is evident in the classic experiments of Heiple on stainless steel [132]. In more detail, the surface tension of pure metals decreases (entropically) with temperature but a surface-active impurity may de-segregate with increasing temperature thereby giving a positive temperature dependence over a non-trivial range of temperature which in turn can reverse the rotation of Marangoni-induced vortices.

The complexities of measuring parameters related to mechanical properties and performance can also be daunting. For example, the variation in YS is often known up to a large fraction of the melting point; however, more detailed and often essential information about creep performance, strain-rate dependencies, and temperature sensitivity is not. Even the elastic response is subject to uncertainty. Although elastic modulus variation with temperature can be fit to simple equations, the value of Poisson's ratio varies strongly, for example, approaching 0.5 near the melting point in many cases.

More accurate and more thorough knowledge of these properties through experimental measurement, possibly augmented with atomistic simulation, is essential for improved PSPP prediction. Section 10.4 summarizes the current status for the measurement of the most important physical properties. For some materials and parameters of interest, new experiments and measurements may be augmented with data from prior work (e.g., research on refractory metals performed in the 1950s and 1960s).

Validation measurements and component testing:
Strong dependencies on local processing conditions may produce location-specific material

behavior and flaws in AM-built components, even after post-build processing. Because existing Q&C approaches rely heavily on coupon-level material testing, a concern exists that such tests may not capture critical behaviors that vary locally throughout a component. This concern is magnified when intentional spatially varying microstructures and compositions are considered. While there are many possible paths forward to address this issue, we will briefly discuss just three examples. First, existing simple coupons can be supplemented by samples that incorporate realistic geometrical features and laser scan paths. The test samples and measurement conditions would likely be developed with the help of CM. Second, CM approaches at the component level may be effective at predicting these local behaviors as described above. Third, Q&C for composite materials has benefitted greatly from the identification of composite layup families that exhibit similar structures and behavior. Extending this concept to part families of AM-built structural alloys may decrease the overall testing burden. All these approaches highlight a need for measurement data to validate CM simulations. The needs for validation and associated recommendations are discussed in more detail in Section 6.

Model validation can occur at several different levels, depending upon the application and the SML. A spreadsheet for assessing SML will be presented in Section 7. For SML 3 or lower, where simulations are used primarily for research or to simply inform Q&C activities, validation requirements should be fairly modest with a large degree of flexibility. For higher SML, where direct impacts on Q&C activities are expected, more rigorous validation methods will need to be developed. For example, at the test sample level, a combination of in-situ build monitoring, NDE, measures of sample geometry and defects, and test-to-failure evaluation could be developed. For high-SML CM simulations, the validation approach must provide high confidence that the simulations accurately reflect reality so that risks can be quantified. For example, for physics-based simulations with coupled, hierarchical models, validation measurements would need to capture the essential physics of the individual sub-models and their interfaces with other sub-models. Currently, such validation measurements are only feasible at great expense for limited materials and processes. One possible solution would be to use these benchmark measurements to validate high-fidelity simulation codes developed on high performance computing (HPC) systems and use these codes as secondary benchmarks for evaluating and calibrating lower-computational-cost simulations and surrogate models.

Ground truth characterization:
As described previously in *Validation measurements and component testing*, the development of location-specific microstructure, material behavior, and defects reduces the applicability of traditional coupon-level material testing. Better inspection technology is required to characterize defect states across a component or coupon over the full range of relevant length scales. Such approaches include NDE, component-level destructive techniques, localized-region destructive techniques, in-situ monitoring approaches, and data fusion approaches that combine information from multiple sources to enable a more complete evaluation of the underlying defect- and micro-structure within a given sample geometry. Example NDE techniques that are currently used include visual inspection, fluorescent penetrant inspection (FPI), computed tomography (CT), eddy current inspection (ECI), X-ray radiography, and ultrasonic approaches. Destructive characterization approaches include mechanical testing with

associated measurements such as digital image correlation (DIC), indentation testing, microstructural evaluation (serial sectioning, scanning electron microscopy (SEM), transmission electron microscopy (TEM), etc.), residual stress characterization using cutting and hole drilling, and automated mini/micro-sample evaluation (mechanical testing and microstructure). When higher-fidelity measurements are required, more expensive and time-consuming approaches are often employed using synchrotron X-rays, neutrons, atom probe tomography (APT), and lower length scale DIC. Another important approach that is discussed in the next sub-section is in-situ monitoring, where defects can potentially be mapped out during the build process without the need for additional costly ex-situ characterization. Of course, rigorous validation of all such approaches is critical. Improvements in all these techniques are required with respect to throughput, cost, resolution, field-of-view, and data fusion. Finally, the development of standards and best practices for these approaches is strongly encouraged.

In-situ measurement and feedforward/feedback control:
Real-time process monitoring during AM manufacturing can be used to eliminate or reduce flaws, identify their locations within a part, improve material properties, and increase build reliability and reproducibility, particularly when coupled with feedforward control (e.g., through model-based predictions) and feedback control (through direct measurement of outputs like melt pool size). For example, infrared (IR) camera data can provide information on melt pool size and shape during a build. CM simulations, together with a database of experimental characterization data, can relate measurable signatures to desired properties, and can also predict effects of process parameters on those signatures. When extended, for example, to two-color pyrometry, real-time measurement of temperature fields becomes feasible [133]. Other data sources, such as magnetic, electrical, or acoustic measurements, can complement optical and thermal information to provide a more complete picture of material state in real time, enabling feedback control systems to shrink process variability and potentially reduce the scope of testing. Significant difficulties remain in identifying the most beneficial measurements, determining the accuracy and precision needed, implementing the required calibration chains, connecting the measurement observables to local process conditions and the resulting material state, and implementing real-time feedback control. Ultimately, the efficacy of in-situ monitoring may be improved with the help of CM tools and standards [134], to the point of providing reliable *probability of detection* for occurrences of specific defect types.

Reducing build variability:
Q&C can be seriously affected by build variability. Variations in the mechanical properties of parts have been observed between different build locations on a single build plate, between different machines from the same manufacturer, and between machines built by different manufacturers. This variability can be contrasted with machining of traditionally processed material, where numerous machine tools from different manufacturers can be used to produce functionally identical parts. Some level of variability for AM-built parts is likely inherent and caused by stochastic processes during the build, but the more systematic variations between different locations on the build plate and different machines is a problem that could be addressed through adequate calibration of CM models, standards, and best practices. The hardest, and most immediate concern is understanding how tightly the process variables need to be controlled to reduce build variability to an acceptable level for a given process or

manufactured component. CM can play an important role in determining these calibration requirements. Build variability/reproducibility is discussed in greater detail in Section 8.2.

5.3.2. Multi-scale and Multi-physics Capabilities

Multiscale model interfacing:
To achieve required levels of computational efficiency for AM process modeling, commercial software available for part-scale predictions of quantities such as residual stress and distortion often rely on simplifications that treat entire individual layers or groups of multiple layers (superlayers) at a time, combined with approximations such as the inherent strain method. These approaches often ignore effects on local thermal history of details such as small geometry features, proximity to interfaces, and laser scan path patterns. However, capturing these local details is expected to be fundamental to predicting meso-scale phenomena such as pore formation, as well as the local grain microstructure and composition.

A well-validated multiscale modeling framework is needed to exchange information in a tightly coupled formulation that efficiently connects part-scale effects to melt pool phenomena, and vice versa, in process-to-structure simulation. Multiscale modeling technologies for structure-to-property relationships, e.g., representative volume element (RVE) models [135], are more mature than those for process-to-structure, but still in need of research to effectively predict part-scale performance. Advanced multiscale methods and accelerated computational techniques, including surrogate models based on PIML, may help bridge this gap. A primary interaction mode for models that operate at disparate length and time scales is via sequential multiscale modeling, where model parameters or model forms identified at the lower (i.e., smaller or faster) scale is passed on to the higher (i.e., larger or slower) scale. Depending on the problem, large discrepancies between the scales of interest pose significant challenges to multiscale modeling. A classic example is interfacing molecular dynamics models to continuum models where the operative time scales differ by 6 to 9 orders of magnitude. This topic has received considerable attention during the past decades [136], yet is likely not sufficiently mature for use in the Q&C domain.

Damage tolerance for AM parts:
By explicitly computing the growth rate of known (via NDE) or anticipated flaws, the field of Damage Tolerant Design enables prediction of the life (generally, fatigue life) remaining to safety critical parts based on the design operating conditions. Flaws, such as microcracks and pores, can develop during the fabrication of the part and grow into cracks due to repeated loading, or fatigue. In AM, microcracks primarily form in materials that exhibit low ductility such as very high gamma prime containing nickel base superalloys, refractory alloys, etc. Such microcracks may be present in high densities; hence, techniques must be developed to prevent or greatly reduce the number and size of such flaws, either by process optimization or by alloy modification, or both. Another factor to consider is the level of anisotropy characteristic of the AM process. As the part is built, grains tend to preferentially grow in the build orientation resulting in crack growth resistance that is dependent on the crack orientation. A third factor relates to the possibility that multiple flaws in a part may interact and merge into a single crack of critical size that leads to premature failure.

Model verification and validation:
In general, commercial CM tools are in the low- to mid-range of readiness level despite often having had many years of development. Although verification of codes against known analytical (mathematical) solutions is typically performed, validation against experimental data is expensive and the software vendors do not have the resources to support this activity directly. As a result, it remains the responsibility of individual users to validate each code against their own (often proprietary) data and to calibrate the models for specific problems. Even where a software vendor has validated their code against experimental data, it is rare that the detailed information is publicly accessible. This means that vendors of CM tools can only validate their codes against the relatively rare instances of publicly released data.

This situation is understandable to the extent that each user has their own domain of application and extrapolation of validated code to a new range of parameter values diminishes confidence. To offset this undesirable state of practice, a recent and very welcome trend is that more authors of papers are posting the associated data in locations such as Mendeley Data and Data in Brief [137,138]. This gradual democratization of data complements the work of government agencies to curate data specifically intended for validation such as NIST's AM Bench and the Air Force Research Laboratory (AFRL) Challenges, see A1.1 CM Efforts and Initiatives. Model V&V is discussed in much greater detail in Section 6.

Uncertainty quantification and propagation:
The quantification of both measurement and modeling uncertainties is critical for assessing the validity of simulation results. UQ for measurements is a highly mature field that has developed over approximately 250 years and forms the basis for *traceability* that allows measurements to be traced back, through an unbroken chain of comparisons, to a national or international standard [139–145]. UQ for computational simulations is less well developed and most simulation packages do not directly support UQ. As described in greater detail in Section 6, the prediction of AM material properties and flaws is subject to both epistemic uncertainty (lack of knowledge of parameters and phenomena) and aleatoric uncertainty (caused by the stochastic nature of an input random variable). A good example is the formation of flaws which arises from a combination of mechanisms, some of which are nearly deterministic (e.g., incomplete melt pool overlap leading to LOF porosity) versus those that are nearly random (e.g., an unusually large spatter particle ejection from a local unstable melt pool). A predictive framework should assimilate simulation and measurement data to provide a probability of flaw formation under given process conditions. Ideally, formation of a failure-inducing flaw is a rare event, meaning that probability prediction requires quantification of the tails of distribution functions, i.e., extreme value statistics and probabilistic approaches to fatigue life. This presents challenges that can likely only be surmounted with a combination of UQ theory and analysis with high-throughput simulation and testing, the use of realistic physics-based assumptions, and an understanding of how uncertainty propagates through the models. A more detailed discussion of UQ is provided in Section 6.

5.3.3. Machine Learning and High-Performance Computing

Machine learning:

Data-driven approaches such as ML can aid in optimizing AM processes and understanding PSPP relationships. ML models based purely on experimental data may be used, for example, to build complex process maps linking process parameters to flaw formation, microstructure, or material properties [146]. This approach may circumvent the need for detailed physics-based models but requires a large amount of training data, and it can be difficult to transfer knowledge between different build machines, material systems, and operating environments. Of more concern, conventional ML approaches can be wildly inaccurate when used beyond the bounds of their training data (i.e., when used for extrapolation). A current area of research, therefore, is to develop techniques that supplement ML models with physical insight and/or detailed simulations (i.e., PIML). Promising approaches include the incorporation of physical laws or constraints into neural network loss functions, the combination of experimental and simulation data in model training, the use of ML to uncover scaling laws and ideal or reduced-order process parameterizations, and the development of ML-based constitutive models to bridge between simulation scales.

Increasing computational efficiency of physics-based models:

In many cases, computational expense rather than model knowledge or availability limits detailed simulation of PSPP relationships. Hence, improvements in computational efficiency are a cross-cutting need affecting nearly all modeling tools discussed in this section. Improvements in hardware and computational algorithms will continue to allow more detailed physics-based models and higher resolution in space and time, resulting in better accuracy and predictive ability. For example, detailed melt pool flow simulations typically require multiple days to solve on large parallel systems; efficiency improvements are needed to allow such tools to be effectively used for process design and optimization. Such approaches are commonly referred to as *reduce-order models* in the sense that ML models do not directly solve the relevant equations (although physics-constrained ML is rapidly advancing) but offer much faster solutions compared to full-field simulations. In some ways, reduced-order models are a more elaborate approach of statistical analyses (also known as data analytics).

Several trends are notable. One is that graphical processing units (GPU) continue to become more powerful and less expensive. This trend is important because many algorithms can be adapted to run on GPUs, including not only the well-known use for ML algorithms but also for scientific computation. For instance, the all-important fast Fourier transform algorithm has been adapted to use GPUs [147]. Another important consideration (albeit, with recent temporal fluctuation) is cheaper random-access memory (RAM) which means that workstations (or clusters or cloud computing) can run larger problems with shared memory among multiple central processing units (CPU), for example, [148]. Trends in readily available hardware provide pathways for vendors of commercial codes to adapt their algorithms and improve the performance of their products [148]. Government-supported thrusts such as exascale computing, e.g., [149], are important for demonstrating future possibilities and for improving algorithms but are less directly impactful on the use of CM tools. However, as mentioned in

Section 1, the U.S. government has developed and deployed exascale-targeted codes for simulating AM processes from the melt pool through mechanical behavior [48].

Data Storage:
The use of CM often requires access to large amounts of data, especially for data analytics, data mining, etc. This need raises several key issues. Current practice in R&D emphasizes an all-encompassing approach to data collection, for example, for machine qualification and alloy development. For production, the typical practice is to identify the data required for operational quality assurance.

Data management plans must optimize return on investment (ROI) while satisfying all requirements for Q&C. Data represent the core of the digital thread for Q&C and are subject to interrogation from multiple stakeholders to verify provenance, accuracy, and completeness. FAIR data practices are recommended to improve evidence-based decision-making processes. All data should be stored alongside all available corresponding metadata. Primary data are useful as core records while metadata are used to supply context to the primary data sources and are instrumental to the FAIR data philosophy. Data security is another major consideration for industrial applications and the FAIR data principles are compatible with these needs.

Presently, there is no universal standard for materials data ontology, though dozens of ontologies have been introduced [150]. This shortcoming is also true regarding schema for capturing all relevant data and metadata. Specific to the AM domain, professional organizations such as ASTM International and ASM International published guidance on common data format utilization to increase efficiency of data-supported decisions [150,151]. Investment in common data formats is a factor for an organization's ROI for the data management plan. Data curation that follows a common data model introduces overhead costs to curate and store records, whether through a creation of a database with tooling to handle read and write operations or through a worksheet approach where data are recorded according to a predefined template. Even though a data management plan that commits to a common data format may not be most convenient for an organization, a systematic approach to manage these challenges in the AM data supply chain offers the benefit of increased efficiency in end-use data retrieval and communication.

5.3.4. Digital Twins and CM4QC

Digital twins (DT) are highly relevant to CM4QC but are used in a variety of different ways in different fields. As stated in the recent National Academy of Sciences (NAS) report on "Foundational Research Gaps and Future Directions for Digital Twins" [152], a "digital twin is a set of virtual information constructs that mimics the structure, context, and behavior of a natural, engineered, or social system (or system-of-systems); is dynamically updated with data from its physical twin; has a predictive capability; and informs decisions that realize value. The bidirectional interaction between the virtual and the physical is central to the digital twin". The scope of such a DT may be limited to a specific part of the entire sequence, e.g., simulation of the 3D printing process in a specific powder bed machine. Or it may be an end-to-end model of the entire sequence to the final part including, for example, printing, heat treatment, and machining. For the purposes of CM4QC, however, the DT should lead to the prediction of a property or performance parameter (e.g., yield stress, fatigue life) that is required for qualification and/or certification. As stated in Conclusions 2-4 of the NAS report, "Methods for ensuring continual VVUQ and monitoring of digital twins are required to establish trust. It is critical that VVUQ be deeply embedded in the design, creation, and deployment of digital twins. In future digital twin research developments, VVUQ should play a core role and tight integration should be emphasized. Particular areas of research need include continual verification, continual validation, VVUQ in extrapolatory conditions, and scalable algorithms for complex multiscale, multiphysics, and multi-code digital twin software efforts. There is a need to establish to what extent VVUQ approaches can be incorporated into automated online operations of digital twins and where new approaches to online VVUQ may be required." In other words, the expectation is that the DT is a complex model comprising multiple sub-models all of which require their own V&V and UQ, together with evaluation of UQ for all the connections.

Again, at the top level, there are several types of DT based primarily on application area. *Component twins* are intended to track parts and components and so the numerical description is generally limited to what is needed to define its function and most of the data concerns the service life along with whatever model, generally basic, quantifies the need for maintenance and detection of faults. *Asset twins* are similar but aim to provide a numerical model of a complete building or machine: in principle such a DT is more likely to be a complex system of models whose aggregate functioning provides predictions of life, need for preventive maintenance, etc. *System twins* model an entire process or system. In most instances these are intended to allow an organization to keep track of an entire organization and the utility is mainly in performance improvement. *Process twins* aim to model business processes or customer experience, again with the aim of improving operations on a holistic basis. A digital twin that is a complete model for an instance of process-intensive manufacturing that uses physics-based simulation is, accordingly, quite far from any of these data-driven DTs. A DT of, say, metals additive manufacturing and the properties of its products could be construed as a specialized *system twin* that provides property predictions as a function of process history. The data input is compact, consisting of information about feedstock, process parameters and expected loadings in service. The data generated in the course of predictions is, however, substantial as the input parameters are propagated through the system of component models.

From a historical perspective, the term *digital twin* was first coined by Dr. Thomas Cruse in 2008 as the title for a DARPA program titled "Stochastic Systems: Transforming System Design & Certification through the 'Digital Twin' Concept" [153]. This was soon followed by discussions involving DTs for aging aircraft led by the USAF and NASA around 2010 [154], and then foundational papers in 2011 by Tuegel et al. [155] and in 2012 by Glaessgen and Stargel [156]. This concept was to create a numerical avatar for each aircraft that could be used to track its condition over time. This approach of avatar-as-digital-twin caught on in part because of progress in CAD, software, data storage, computer capacity, in-situ sensing for health monitoring/management, etc. Well before this, however, there was interest in modeling manufacturing processes, including materials production. Crumbach et al. [157], for example, published on "Through-process texture simulation for aluminum sheet fabrication" which outlined a model for predicting microstructure and anisotropy resulting from typical thermomechanical processing of industrial Al alloys. This, at the time, was a relatively complete approach to a specific aspect of materials manufacturing but not directly connected to properties.

In recent years, the increasingly digital nature of manufacturing has enabled use of numerical avatars at the materials level (as opposed to systems such as engines and vehicles). Metals AM, being intrinsically digital in nature has attracted direct interest with papers directly addressing the creation of (numerical) digital twins with full computational approaches to predicting microstructure emerging from metals AM [158]. There are now active research projects such as the NASA-supported Institute for Model-based Qualification and Certification of Additive Manufacturing (IMQCAM) [159]. To a large extent, a numerical digital twin (of metals AM and other processes) that has the capability to predict key materials properties such as fatigue and that is fully validated, with quantified uncertainties, represents the federated approach to computational materials that is most likely to be useable for accelerating Q&C. In other words, a fully developed DT for metal AM can be the realization of CM4QC that is the implementation that engineers need for day-to-day use.

5.3.5. Standards

Another critical component of the AM Q&C ecosystem is technical standards developed by various SDOs and consortia [9]. Such standards have many uses, such as communicating guidance and best practices, specifying requirements (both customers' and regulatory), defining test methods and protocols, and documenting technical data. When properly implemented, these standards may carry several benefits, including accelerating adoption of new technologies, enabling trade in global markets, and ensuring human health and safety. Standardized measurement procedures and documentary standards are rigorous and broadly accepted and can therefore play a critical role for Q&C by providing confidence. Also, certifying bodies and government regulatory agencies may reference some of the publicly available standards in their requirements, or as acceptable methods of compliance.

In the U.S., standards development is conducted through voluntary participation and consensus. Several standards bodies and industry-government consortia have AM relevant activities, including ASTM International Committee F42 on Additive Manufacturing Technologies, International Organization for Standardization (ISO) Technical Committee 261 on Additive Manufacturing, ASME Y14 Subcommittee 46 - Product Definition for Additive Manufacturing, SAE International Aerospace Material Specifications for Additive Manufacturing (AMS-AM), European Committee for Standardization (CEN) Technical Committee 438 on Additive Manufacturing, Metallic Materials Properties Development and Standardization (MMPDS), and many more. A key summary and roadmap for AM technical standards [160] and a corresponding gaps progress report [161] have been developed by the Additive Manufacturing Standards Collaborative (AMSC) initiative and are available online. Section 2.3 of the latter reference describes standardization gaps for Q&C. Many of these identified gaps are highly specific and relate to narrow application areas that are not directly relevant to the CM focus. Here, discussion will center on standards for VVUQ of CM models as they relate to PIMs for aviation applications.

While some V&V standards already exist (e.g., [162] and [163]), these are limited to single-scale computational modeling approaches such as FEA and CFD. Much work is required to establish V&V standards and best practices that address the multi-scale and multi-physics simulations typical for AM PSPP needs. Similarly, UQ approaches and requirements for physics-based simulations have been studied extensively over the past 20+ years, and many organizations are pursuing development of standards and best practices for their use (e.g., DOD, NASA, ASME, the American Institute of Aeronautics and Astronautics (AIAA), the International Organization for Standardization (ISO), the Institute of Electrical and Electronics Engineers (IEEE), Sandia, and Los Alamos National Laboratory (LANL)). However, as with the V&V standards, most of this work focuses on single-scale and limited-physics modeling approaches. UQ standards and best practices need to be extended to multi-physics, multi-scale simulations to be relevant for Q&C within the context of CM applications to PIMs. Two recent review papers on UQ discuss many of these issues in greater detail [164,165]. General descriptions of current VVUQ practices are provided in Section 6 and VVUQ requirements for different SMLs are discussed in Section 7.

Another relevant lack of standards is in the area of VVUQ for data-driven approaches. Code verification, model validation, and model uncertainty quantification for data driven approaches are fundamentally different from more traditional physics-based modeling. This topic is discussed in Section 6.5.3.

Section 6 Key Elements & Associated Methods for Computational Materials Verification, Validation & Uncertainty Quantification

6.1. Introduction

Rigorous V&V is needed to establish trust in CM-informed approaches to Q&C. In this context, as defined in the Glossary (Appendix VII), *Verification* is the process of determining the extent to which a model or simulation is compliant with its requirements and specifications as detailed in its conceptual models, mathematical models, or other constructs. *Validation* is the process of determining the degree to which the model is an accurate representation of corresponding physical observations from the perspective of the intended uses of the model. The predominant distinguishing feature between *verification* and *validation* is that validation requires comparison with physical experiments whereas verification does not. Basically, verification always refers to the *correctness* of the simulation itself, whereas validation refers to the capability of the model to reproduce physical experiments. The key takeaways from V&V are summarized below.

- V&V must be based on the *intended use*, and validation for one intended use does not automatically extend validation to other uses. Each use must be examined independently.
- UQ is an essential element in both the simulations and experiments and should be addressed explicitly. The term VVUQ is sometimes used to indicate the essence of UQ within the V&V framework.
- The validation experiments should be designed in consultation with the modelers. These experiments are likely to be decidedly different from traditional experiments of *proof-of-concept* and *discovery*, as described in Section 6.2.2.
- Documentation is a key output of the V&V process as it provides a complete record of all steps of the V&V process and justification for important decisions. That is, in addition to details, it contains the *why* of the process. In addition, since VVUQ is a continuous process, complete documentation provides a well-defined starting point for subsequent validation projects.
- The validation of a model for an intended use is a systematic process that depends upon the chosen validation metric and validation threshold.
- The use of a validated model to make predictions outside of a validated domain where no experimental data are available should be used with caution and consideration of the risks and consequences involved.
- V&V can be conducted for any tier of the system: subsystem, component, or unit problem and different response quantities and validation metrics can be defined at any tier of the hierarchy.
- Validation does not imply that the experimental data are always more accurate than the computational results. Experimental uncertainty estimates may be very high, and unknown bias errors can exist in the experimental data.
- The data used for calibrating a model cannot be used for validating the model.

The information provided here is a summary of the V&V process. A general framework for this process is provided in Section 6.2, with subsections on 6.2.1 Code Verification, 6.2.2 Design of Validation Experiments and Preliminary Calculations, 6.2.3 Calculation/Solution Verification, 6.2.4 Uncertainty Quantification of Simulation Results, 6.2.5 Uncertainty Quantification for Experimental Results, and 6.2.6 Validation. Documentation needs are discussed in Section 6.3, followed by a brief discussion of predictive capabilities in Section 6.4. Section 6.5 provides a summary of UQ, with 6.5.1 providing an overview of model UQ, 6.5.2 narrowing the focus to UQ for AM processes, and 6.5.3 describing the current state of knowledge for VVUQ of data driven models.

6.2. Framework

The framework for conducting V&V is shown in Figure 6.1 and follows the outline presented in references [162] and [166]. The emphasis of the framework is twofold: a) the design of the validation experiments is conducted as a *joint* effort between the simulation team overseeing the mathematical modeling and simulations and the experimental team overseeing the physical modeling and experiments, and b) UQ is an essential element of both computations and experiments. As shown in Figure 6.1, six steps are called out using numerical values 1-6. The sequence of suggested steps is:

1. Code verification
2. Design of validation experiments and preliminary calculations
3. Calculation/solution verification
4. UQ for the mathematical model
5. UQ for the experimental results
6. Validation

Clearly there is some flexibility in the sequence of events (for example 4 and 5 can be conducted in parallel); however, the key concept is that design of the validation experiments should be done in concert with the development of the computational model and with the intended use in mind.

Figure 6.1 Framework for conducting V&V. Adopted from references [162] and [166].

6.2.1. Code Verification

Code verification deals with the mathematical correctness of a numerical solution (*the equations are programmed correctly*). Code verification does not address whether the mathematical model reflects reality; that is the subject of validation. It should be clear that verification for one intended use does not automatically extend verification to other uses.

Guiding principles behind code verification include the following:

- Software can be thought of as another kind of experimental apparatus and should be developed, checked, and used as carefully as any physical apparatus.

- Code verification involves finding and removing mistakes in the source code and in numerical algorithms and improving the software using software quality assurance practices.
- Verification often utilizes knowledge of the exact solution to a problem of interest or the method of manufactured solutions to create a problem for which an analytical solution exists.
- Code verification implies the use of software best practices [167]. Example best practices include: use of a version control system (e.g., Git), producing a modularized code, adding assertions to check operations (e.g., unit testing), use of an issue tracking tool, documenting the design and purpose of the code in addition to the mechanics, embedding the documentation for the software within the software (e.g., Javadoc), and finally, using code reviews.
- Code verification can be conducted using a variety of criteria including: simple tests (e.g., solution obeys symmetry, energy conservation), code-to-code comparisons for independently-developed codes, discretization error quantification (quantify the error with respect to a known exact solution for a discrete mesh and time step), convergence tests (assure convergence of the QOI(s) as the mesh and time step are refined), and order-of-accuracy tests (examine that the rate of convergence matches the theoretical values) [168].
- Code verification is primarily the responsibility of the software developer; however, evidence that code verification was rigorously conducted should be required by code users.

6.2.2. Design of Validation Experiments and Preliminary Calculations

Validation experiments should be designed explicitly to validate computations and are different from traditional or discovery experiments. For traditional experiments, e.g., a proof test, the customer is typically the design group or project group. The emphasis is normally on high-level measurements of system or subsystem performance. In discovery experiments, the emphasis is on observing and understanding physical phenomena, and/or building or improving mathematical models of physical phenomena. For validation experiments, computational simulation becomes the primary customer of the experimentalist, not the design, or project group. As such, validation requires close cooperation between the modelers and experimentalists. Required measurements now include all initial conditions, boundary conditions, and auxiliary conditions needed for the computer model. There is an important emphasis on estimation of measurement uncertainty.

Communication between the modelers and experimentalists is also crucial to determine levels of experimental uncertainty required for the validation measurements. Typically, the requirements of measurement accuracy and precision determine the specific measurement methods that are required.

As a minimum, validation should encompass the following tasks:

1. Define the intended use and the QOI.
2. Define the purpose and intent of the experiments.

3. Provide preliminary model inputs and simulations.
4. Describe methods for measuring required model input data.
5. Develop and prioritize approaches for measuring QOIs.
6. Maintain and preserve records of all associated datasets and procedures and assumptions.

6.2.3. Calculation/Solution Verification

Solution verification is the quantification of the numerical error in a computer solution. In this case, an exact solution is not known. Solution verification must be performed for every simulation that is sufficiently different from previously verified solutions and is primarily the responsibility of the software user or analyst. Solution verification is commonly ignored by code users and decision makers; however, this is a serious mistake since evidence of solution verification should be required by decision makers.

There are three main aspects of solution verification [168]:

1. Verification of input data:
   Ensuring correct input files; questioning the choice of computational domain, decisions regarding meshing strategies, tabulated data, boundary conditions, physical parameters, fitted parameters, etc.; archiving the important data
2. Numerical error estimation of the solution:
   Including discretization error, iteration error, round-off error, and statistical sampling error for stochastic models
3. Verification of post-processing tools:
   Ensuring that the correct post processing steps are taken, e.g., having a checklist for the analyst to process

6.2.4. Uncertainty Quantification of Simulation Results

UQ is the process of quantifying uncertainties associated with model calculations of physical QOIs, with the goals of accounting for all sources of uncertainty such as parameter, environmental, model form, etc., and quantifying the contributions of the specific sources to the overall uncertainty through the use of sensitivity analysis. UQ traditionally uses probability theory to estimate probabilities, statistical moments such as mean and variance, cumulative distribution functions, probability density functions, etc. The use of UQ for process intensive applications (such as AM) will be discussed in greater detail later in this section.

6.2.5. Uncertainty Quantification for Experimental Results

Experimental uncertainties can originate from experimental equipment and facilities, measurement techniques, diagnostics, physical fluctuations, and/or post-processing approaches. UQ of experimentally based uncertainties is the process of quantitatively characterizing the uncertainty (both random and systematic) for a measured QOI, based on all necessary inputs and parameters involved in executing an experiment that is employed to approximate physical phenomena associated with the predictions of the simulation. Rigorous, internationally accepted methods for evaluating and propagating measurement uncertainties have been established by the Bureau International des Poids et Mesures [139–145].

6.2.6. Validation

Validation of a computational model refers to the process of determining the degree to which the computational model is an accurate representation of corresponding physical reality from the perspective of the intended uses of the model. Validation thus involves the quantitative comparison of simulation results to experimentally measured values, and a model is considered *validated* within regions of the parameter space where agreement between simulation and measurement is sufficiently high for the intended use case. It should be clear that validation for one intended use does not automatically extend validation to other uses, and it is not appropriate to use experimental data in model validation that has already been utilized to calibrate the model.

The following tasks should be accomplished during the validation process:

1. Review boundaries of applicability of the model.
2. Compare computational outputs to experimental results and their uncertainty ranges.
3. Quantify validation metrics and produce data visualizations.
4. Define validation limitations and assumptions.
5. Allocate resources for developing validation data and metrics.
6. Document and disseminate validation metrics among all stakeholders.

6.2.6.1. Validation Metrics

The determination of the validation of a computer model for the intended use is based on a chosen validation metric and threshold value. As such, the choice of the metric and acceptable threshold value is a critical component of validation of a model. These quantities are subjective; hence, validation itself will always be subjective. At present, there are many phenomena with no widely accepted validation metrics; however, there are characteristics that a validation metric should contain [169,170]:

- A metric should be a *quantitative* measure of the agreement between predictions and physical observations. A metric should also be *objective*, which means that given the predictive and experimental datasets, the metric will produce the same assessment for every analyst independent of their individual preferences or biases.
- Calculating the validation metric is separate from the judgement of whether or not the model is acceptable. The judgment involves other considerations such as the prediction domain and performance risk, and potentially public policy.
- The uncertainties resulting from both computer models and experiments need to be considered, together with the correlation among multivariate responses. In other words, because the computer prediction and experimental measurement are both uncertain, the metric must operate on these uncertainties. Ideally, the value of a

stochastic validation metric should degenerate to the value from a deterministic comparison between scalar values when uncertainty is absent.

- Additionally, the validation metric should provide a statistical confidence level associated with the amount of available experimental data.
- A validation metric should differentiate between models containing greater and lesser amounts of uncertainty. For example, its value should not be improved if the analyst introduces additional sources of uncertainty into modeling, e.g., widening the probability distribution of a model parameter to gain a greater chance of encompassing physical observations. The same is true for the experimental 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. This last feature is critical from the viewpoint of engineering design.

6.2.6.2. Model Calibration

Model calibration is the process of utilizing measurement data to determine appropriate values of model parameters to improve the agreement between predictions and measurements, also known as *model tuning*. It is essential to ensure the differentiation between validation and calibration steps, that is, the data used for calibration should not be used for validation.

6.2.6.3. Validation Challenges

Validation needs to address technical issues such as insufficient understanding of a complex physical process, inability to measure key system responses or large measurement uncertainties in experiments, and high dimensionality of model outputs and measurements, e.g., electron backscatter diffraction (EBSD) maps. Challenges encountered while conducting the validation process can illuminate and help prioritize areas that need further investigation.

6.2.6.4. Extensions to AM processes

The V&V framework, as described in 6.2, directly applies to CM4QC although there exist discipline-specific components. The ASME Committee on Verification & Validation in Computational Modeling and Simulation has a subcommittee on advanced manufacturing (V&V 50) for manufacturing processes, including AM. Some of the V&V and UQ activities related to AM could rely on the standards published by the V&V 10 and V&V 20 subcommittees (for solid mechanics models, and fluid mechanics and heat transfer models, respectively) [162,163].

6.3. Documentation

A critical output of a V&V exercise is the documentation of the process. This information should be sufficient such that the computational and experimental results are *reproducible* by others but, in addition, as described in reference [171], *"the essence of V&V documentation is to provide the rationale for the selected physics equations, list assumptions, define metrics, explain the relationship between numerical and experimental results, and catalog uncertainties."*

Ultimately, the documentation should provide evidence for the conclusion whether the model is validated or not for its intended use. This documentation also allows subsequent validation efforts to have a well-defined starting point.

The following is guidance for documenting the activities and evidence supporting the credibility of the computational model as discussed in references [162]:

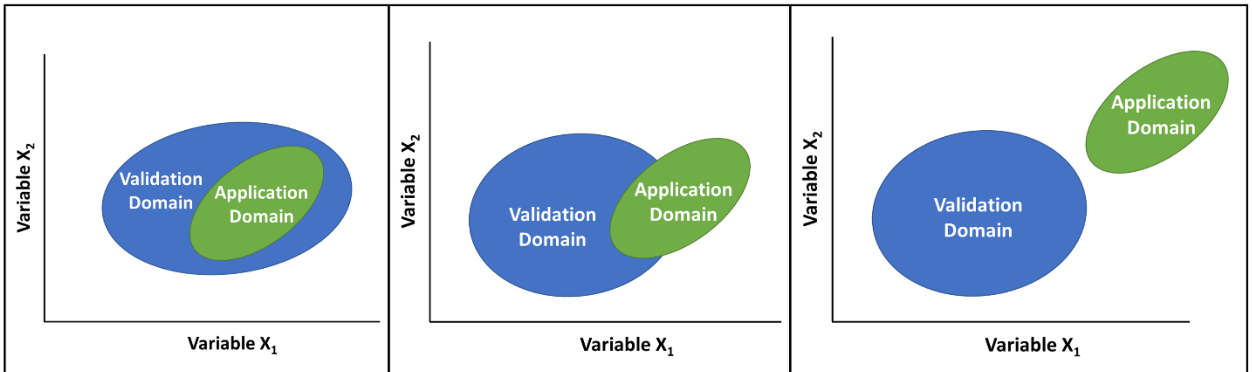
- *Background* - information that describes the device, material, process, or system feature(s) being modeled. This may include information about the basic operation of the device, process, or system. It may also include a description of the application as it relates to the intended use.
- *Intended use of the Computational Model* - a description of the intended use for the computational model that includes information regarding the decision that is being informed by the computational model results, as well as a description of any other sources of supporting evidence that are informing the decision.
- *Computational Model Details* - documentation describing the relevant details of the computational model for the intended use. This information includes all assumptions, boundary conditions, material parameters, and numerical algorithmic parameters/settings.
- *Model Risk -d*ocumentation of the overall model risk, including an evaluation of the computational model influence and decision consequence, and an overall statement regarding model risk determination.
- *Model Credibility Assessment* - documentation of the credibility assessment activities, including a description of the goals for the credibility factors, the activities conducted, and the evidence supporting the credibility of the computational model. This includes the relevant details of the computational model and each comparator used for the *V&V* activities.
- *Conclusions* - a summary of the overall credibility of the computational model for the intended use as evidenced by the credibility activities.

6.4. Predictive Capability

Prediction is often realized through computational models that foretell the state of a physical system under conditions for which the computational model has not been validated nor calibrated [172]. Issues that might affect the confidence in a prediction, i.e., estimation of uncertainty in a prediction, include:

- What is the measure of agreement between computation and experiment for experiments near the prediction, more specifically, what is the value of the validation metric?
- How different are individual experiments in the validation database from the prediction of interest?
- What additional possible sources of uncertainty are introduced in the prediction of interest?

The relationship between validation and prediction can be classified into three groups as shown in Figure 6.2, below [173]. The relationship between the domains of validation and the application is shown schematically on a two-dimensional scale of arbitrary variables X_1 and X_2. The confidence of model predictions is highest at the validation points and decreases away from the validation points. Hence, the confidence of the predictive model is decidedly different for each case. The confidence should be carefully weighed against the consequences for each case.



Interpolation – Complete overlap of application domain and validation domain	**Well-founded inference** – Partial overlap of application domain and validation domain	**Weak inference** – No overlap of application domain and validation domain

Figure 6.2 Relationship between Validation and Prediction. Adapted from [173].

6.5. Uncertainty Quantification

UQ is a fundamental aspect of the V&V process (often designated VVUQ) for all disciplines [162]. A summary of some of the issues pertaining to AM-built parts is discussed here.

AM products can show significant variability in a variety of metrics, including geometric accuracy, roughness, microstructure, flaws, strength, and fatigue properties. The models to predict these quantities are also affected by multiple uncertainty sources. Thus, UQ is a critical component of the CM toolchain in that it provides quantifiable confidence in the predictive capability of computational simulations. Consequently, UQ is an essential component of the V&V process. Despite this criticality, our current assessment is that UQ is either not performed as a part of standard assessment of predictive capability of the existing CM capabilities or is performed in a narrow sense using local parametric sensitivity analysis or by testing effects of incorporating various physical processes in the simulation. While this information provides valuable insights, it is likely not sufficient to build sufficient confidence for Q&C.

6.5.1. Overview of Model Uncertainty Quantification

In UQ, there needs to be explicit recognition and quantification of two types of uncertainty: *aleatory* uncertainty, which involves the natural variability of physical quantities, and *epistemic* uncertainty, which is lack of knowledge arising from either data uncertainty (e.g., sparseness, imprecision, omissions, and measurement and processing errors) or model uncertainty (unknown model parameters, numerical errors, and model form errors).

Some of the AM model inputs (e.g., laser power, laser velocity, etc.) and model parameters (e.g., thermal properties, mechanical properties, etc.) can have both aleatory and epistemic uncertainty, i.e., variability across different specimens as well as unknown values in any one specimen.

In such cases, it is necessary to separate the contributions of aleatory and epistemic uncertainties to clearly interpret the model validation and UQ results and to support decision-making for uncertainty reduction (i.e., model refinement versus additional measurements) by identifying the dominant uncertainty sources through sensitivity analysis [174].

UQ can be performed for both forward and inverse problems. In the *forward problem*, the various uncertainty sources are propagated through the system model to quantify the uncertainty in the predicted values from the model, whereas in the *inverse problem*, the model parameters and their uncertainty are estimated based on the comparison of model prediction and real-world observations.

6.5.2. UQ for AM Processes

UQ in the AM process presents significant challenges. It requires a quantitative understanding of the variabilities in the model input parameters, knowledge of correlations between these input parameters, careful quantification of the consequence of modeling choices made (i.e., model form uncertainty) for computations, and finally, aggregation of these uncertainties through uncertainty propagation methods to obtain the uncertainty in the model output. An additional need is the collection and availability of a sufficient amount of measurement data to allow quantification of input uncertainty. Although certain stakeholders have access to specific data, such as microstructure, melt pool, and thermal history, restrictions on data access and sharing pose barriers to assessing uncertainty for the broader community.

Another challenge is that VVUQ methods have primarily focused on quantifying model errors and prediction uncertainty of physical systems that involve individual physics disciplines, such as solid mechanics, fluid mechanics, and heat transfer. However, when applying these methodologies to AM, challenges arise due to the involvement of multi-physics, multi-scale interactions, and data-driven (e.g., ML) models based on experimental data [164].

An additional challenge is that physics-based PSPP models of AM are computationally demanding, especially for realistic part sizes and geometric complexity. Much of the research literature has considered very small part sizes and regular shapes. VVUQ activities involve multiple runs of the physics-based models. Thus, surrogate models are often built to replace the original physics-based models to help carry out some of the UQ activities (such as model calibration) at affordable cost. Quantities that are predicted and measured (such as temperature) vary over space and time, which causes the additional challenge of high dimensionality. Solutions have been proposed for many of the aforementioned UQ issues [175]; however, they have been demonstrated only with small part sizes. Thus, some important needs in UQ for AM are:

- Scaling up of UQ computational techniques and demonstration of accuracy and efficiency in applications to realistic part sizes
- Addressing the complexity and quality of measurements and quantifying their uncertainty

- Systematic aggregation of uncertainty resulting from multiple heterogeneous sources.

6.5.3. VVUQ of Data-Driven Models

As discussed in Section 5.3.3, the difficulty and complexity of physics-based modeling regarding some aspects of the AM process have led to the development of data-driven empirical models. Such data-driven models do not necessarily include physics, or first principles. Instead, they are trained with input and output data and effectively *learn* what inputs create corresponding outputs. Integrating data-driven methods with simulation-driven statistical approaches offers viable avenues for conducting UQ across different types of simulations in metal AM. Specifically, data-driven techniques can be employed to address and quantify the impacts of *unresolved* scales and physics in the simulation, treating them as black box (aleatoric) uncertainties. Simulation-driven UQ could subsequently be performed by considering these uncertainties. Data-driven ML models, including PIML models, are being developed at a steady rate to predict various quantities of interest in AM.

ML models differ from physics-based mechanistic models, leading to differences in the concepts and methods of V&V and UQ. Verification, in particular, presents unique challenges. In the context of physics-based models, verification entails two activities: code verification, which verifies the correctness of the computer code, and solution-approximation error. The latter activity involves measuring the errors that arise from numerically solving the governing differential equations derived from fundamental physics principles such as discretization error (resulting from discretizing the continuum domain, as seen in FEA and CFD), truncation error (associated with reduced-order models), and surrogate model error (arising from substituting the original physics model with a surrogate model). It is important to note that these errors are specific to physics-based models.

ML models can be constructed using empirical data or simulation data generated by physics-based models. The present section emphasizes the development of ML models based on empirical data.

In the construction of an empirical ML model, the objective is to fit the available data, which eliminates the occurrence of solution approximation errors in solving differential equations or model reduction errors (truncation errors). As a result, the conventional understanding of *verification* does not apply in this context.

When building and evaluating ML models, it is common to quantify three types of errors: *training error*, *test error*, and *holdout error*. (In some ML publications, these three terms are alternatively referred to as *training error*, *validation error*, and *testing error*). These errors are computed by comparing the model's predictions to the observed data and assessing the residuals using a variety of metrics. It is standard practice to partition the available data into three sections and perform cross-validation using the training and test sections. This involves swapping or shuffling data between the training and test sections to minimize overfitting and reporting an average error measure from multiple partitions or *folds*. The holdout error provides insights to the practitioner regarding the extent of overfitting. Quantifying the first set of error values could be considered as a form of *verification* for ML models, while quantifying the holdout error serves as *validation*. However, it is important to note that the ML literature does not typically use the term *verification*. Therefore, it is advisable to reserve this term for physics-based models and avoid confusion in terminology when referring to ML models. In general, *verification* evaluates where the model meets specified requirements, and the requirements could be stated in terms of error magnitudes or percentages in ML models. Such error requirements could include holdout errors as well, thus further confusing the distinction between validation and verification for ML models. For practical implementation, it might be more valuable to define formal requirements for an ML model and check whether those requirements are met, and not get stuck in arguments about whether it is verification or validation.

A closely related task is the quantification of uncertainty in the predictions of ML models. The ML model inherently produces a residual, which measures how well the model fits the available training data. It is crucial to assess whether this residual follows a normal distribution with a mean of zero; various techniques exist to quantify the variance of the residual.

On one end of the spectrum, there are simple regression models, where the variance of the residual can be analytically computed using a matrix-based formula. On the other end exist decision tree and neural network models with multiple layers and numerous nodes per layer. In such cases, uncertainty is quantified using the dropout technique. In the dropout technique, multiple sub-models are trained by randomly dropping a selected percentage of nodes and/or variables. The uncertainty in the model prediction is then quantified by considering the ensemble of predictions obtained from these sub-models [176,177].

The process of validating an ML model shares similarities with that of validating a physics-based model, and various relevant testing metrics come into play including classical (e.g., t-statistic and chi-square) and Bayesian methods [164]. In addition, when comparing multiple ML models in terms of their fit to the same data, information-theoretic metrics for model selection are available. These metrics, such as the Akaike information criterion, Bayesian information criterion, and minimum description length, consider both the model error and the model's complexity, typically measured by the number of parameters. These metrics penalize models with a larger number of parameters [175].

One important consideration in using ML and PIML models is that they should not be extrapolated outside the range of the data that was used to train them. This means that the training data should cover the range of operating conditions in which the ML models will be used. This consideration also applies to the question of transferability of ML models from one AM machine to another, i.e., where the training data is generated using experiments with one AM machine whereas the usage of the trained ML model might be with another AM machine. Thus, the training data should have adequate coverage of the actual operating conditions and machine-to-machine variations. The amount of data used for training and evaluation of the ML model is an important concern, both from the point of view of building confidence in the model and from the point of view of cost of acquiring the data. These two are opposing concerns, thus a trade-off might be needed.

While the above metrics are commonly applicable to ML models constructed solely with empirical data, caution is needed when applying them to ML models built using data generated by physics-based simulation models, such as surrogate models. Empirical data inherently contain noise due to natural variability in measurements, environmental factors, and other physical quantities. Conversely, physics-based computational models are typically deterministic, meaning they consistently produce the same output value for a given set of input values. Certain computational models utilize a random number generator, introducing a built-in variance that can be measured. Even though they are widely reported as measures of surrogate model accuracy in the literature, the effectiveness of metrics such as cross-validation error may not be clear for computational models that contain a built-in variance utilizing a random number generator.

This issue becomes more complicated in the case of PIML models. Various strategies for constructing PIML models have been documented [178]. These strategies include:

1. Incorporating physics constraints into the loss function of the ML model constructed using empirical data
2. Building physics constraints like symmetries and invariances into the structure of the ML model
3. Building the ML model exclusively using data generated by a physics-based computational model (essentially surrogate modeling)
4. Utilizing the ML model from (III) as an initial model and updating it with empirical data

These different strategies are employed based on the availability of data, whether empirical or derived from physics-based simulations. The efficacy of model evaluation metrics available in the regression literature has not been thoroughly investigated.

The preceding discussion has primarily addressed numerical prediction models, but it is worth noting that ML has also been extensively employed in the development of classification models. These models have been reported in AM for various purposes, including flaw detection. Evaluating classification models involves utilizing a distinct set of metrics, such as accuracy, precision, receiver operating characteristic curve, and more. However, the same concerns mentioned earlier regarding the effectiveness of evaluation metrics (for ML models) persist when physics-based computational models are utilized to generate training data for the ML model in the context of classification models.

The ASME Committee on VVUQ recently established a subcommittee on VVUQ of ML models (VVUQ 70) whose purpose is to develop standards for the VVUQ of ML models.

Section 7 Computational Materials Simulation Maturity Level (SML) Assessment Framework

7.1. Introduction

As described in Section 3, industry is looking toward CM engineering as a potentially transformative technology for decreasing the testing and measurement burden of Q&C for aviation applications of metal AM. In Section 5 we explored how industry is already using computational materials engineering capabilities for such applications and how mature those capabilities are with respect to V&V. Here, we provide a methodology for assessing the SML of simulations used for Q&C of AM-built components for the aviation industry.

This SML assessment framework is based on an earlier development by Cowles et al. [179,180] of an ICME tool maturity level assessment guide. Other developments that influenced the current work are a Sandia study by Oberkampf et al. [181] on modeling and simulation maturity, with a strong UQ component; the ASME *Standard for Verification and Validation in Computational Solid Mechanics* [162]; and a recent publication, *Accelerating the Broad Implementation of Verification and Validation in Computational Models of the Mechanics of Materials and Structures* [166].

The differences between these earlier developments and the current work are driven primarily by the specific focus of this document. Looking at the original Cowles assessment guide, the ICME application space was described as "aerospace materials and processes engineering — including materials design and development, process modeling, and prediction of material behavior" [179]. The current focus is restricted to a narrower range of process conditions (PIM technologies with immediate application to AM), but a considerably larger application space including material and product development, qualification, certification, and life cycle prediction with performance risk assessment (see Figure 3.1 and Figure 3.3). More broadly, although the primary emphasis is on aviation AM applications, this SML assessment guide should be applicable whenever simulations are integral to Q&C, independent of the specific target area or build process. In addition, more modern concepts such as the use of FAIR data principles [14,15], validation of coupled multi-scale, multi-physics models through hierarchical model validation [13], and UQ and V&V for data-driven modeling approaches are included. Overall, the UQ and V&V aspects of this roadmap are well aligned with the content of references [162,166,181] and these topics were discussed in detail in Section 6, Key Elements and Associated Methods for Computational Materials V&V.

The SML assessment framework is presented in the form of a spreadsheet, where the columns describe assessed criteria and the rows describe requirements for achieving five different levels of maturity, with level 1 being the lowest maturity level and level 5 being the highest. Thus, each cell of the spreadsheet includes a brief description of the requirements for achieving the row-specified level of simulation maturity. The complete spreadsheet is provided in the Supplementary Materials.

Table 7.1 SML descriptions provides descriptions of the five SMLs. These levels and level descriptions are mostly unchanged from the original formulation by Cowles, et al. [179], with just minor modifications required for the change in focus. These SML descriptions provide very short specifications for the SML along with a description of activities that can be supported. For example, a simulation with SML 1 can provide some physical insight but is not suitable for Q&C activities. In contrast, a simulation with SML 4 or 5 can be used to provide guidance and confidence to both design and development activities.

Table 7.1 SML Descriptions

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.

A list of the assessment criteria is given in Table 7.2 SML assessment criteria. These are substantially modified from the earlier formulation by Cowles et al. [179]. The earlier assessment criterion *Model Rationale, Basis, and Definition* has been replaced by a more tightly defined criterion *Application and Model Definition*. In addition, the current formulation uses individual columns for *Range of Applicability* and *Uncertainty Quantification* whereas the earlier formulation incorporated these as a single criterion. Similarly, *Model Validation* and *Risk Assessment* are now separated. The former approach had the advantage of producing just six evaluation criteria, but we determined that combining multiple, essentially independent, criteria together made it difficult to develop clear metrics and requirements for the different maturity levels.

Table 7.2 SML Assessment Criteria

Spreadsheet Column	Assessment Criterion
C	Application and Model Definition
D	Range of Applicability
E	Supporting Data
F	Model Verification
G	Uncertainty Quantification
H	Model Validation
I	Performance Risk Assessment
J	Documentation

It is important to recognize that a given software package can have different SML's for different applications. For example, if substantial validation data exist for a particular material and set of process conditions, then applications whose range of applicability fall within these limits may have substantially higher SML than those that fall outside. Thus, the target application is a key determinant for the resulting SML, and the assessment criteria were written with this in mind. Because simulation software vendors cannot be expected to provide supporting data, UQ, and model validation for all conceivable applications, achieving high SML for any particular application must be a shared responsibility between the user and the simulation software developer.

Another important topic is how to assign a single SML to a simulation when maturity is uneven across the assessment criteria. In general, an assessed SML is determined by the *lowest* maturity level over the full range of criteria. For example, if a given simulation is highly developed for all criteria except for Performance Risk Assessment, then the simulation SML is determined by the Performance Risk Assessment criterion.

In this section, the SML assessment criteria will be discussed within individual subsections and detailed explanations of each cell of the spreadsheet will be provided in Appendix III. An abbreviated documentation activity tracking guide that is adapted from Ref. [179] is provided in Appendix IV, and is included as a worksheet within the SML spreadsheet.

7.2. Application and Model Definition (Column C)

The first step in implementing a meaningful CM simulation is to define the intended application. As mentioned in the previous section, a given simulation package can have different SML's for different applications, so it is important to provide an adequate definition. Many of the assessment criteria described in the SML spreadsheet refer back to this application. Another critical step is to define the models that are required along with the model inputs and outputs. Taken together, these definitions comprise SML 1 for Application and Model Definition as shown in Table 7.3.

SML 2 takes the model definitions further by defining all significant sub-models along with their inputs and outputs. This set of hierarchical models comprise the entire set of coupled simulations required for the intended application. Although not explicitly mentioned in the cell descriptions shown in Table 7.3, the interfaces between the simulations should also be defined at this SML level. These interfaces may range from simple passing of parameters to complex bi-directional information flows between sub-models at greatly different temporal and spatial resolutions.

Once the models, sub-models, and model interfaces have been defined, there should be increased understanding concerning how well the simulations can address the intended application. For SML 3, this deeper understanding is used to refine the definition of the recommended application and define the simulation limitations more accurately. For higher SML levels, the application definition and simulation limitations need to be updated given the corresponding higher level of verification, validation, and UQ. Although there is a strong connection between "Application and Model Definition" and "Range of Applicability," they are distinct; the "Application and Model Definition" addresses definitions and general model limitations whereas the "Range of Applicability" primarily addresses the acceptable ranges of input parameters.

Table 7.3 Application and Model Definition SML Descriptions

Maturity Level	Description
1	Application intent defined. Models defined. Model inputs and outputs defined.
2	Significant sub-models defined. All sub-model inputs and outputs defined.
3	Recommended applications and limitations defined.
4	Recommended applications and limitations updated.
5	Recommended applications and limitations updated (suitable for all intended use cases).

7.3. Range of Applicability (Column D)

The Range of Applicability for a simulation must be defined with respect to the intended application as specified in Application and Model Definition (Table 7.4) and draws heavily upon many of the other columns as described below. The methods used to assess the appropriate range of applicability is left to the user and may include comparison with analytical results, information in the literature, comparison with previously validated simulations, etc. However, for Q&C activities it is strongly recommended that SML-appropriate model verification, model validation, and UQ be conducted as described in Section 7.5 Model Verification (Column F), 7.6 Uncertainty Quantification (Column G), and Section 7.7 Model Validation (Column H), respectively. Section 7.8 Performance Risk Assessment (Column I) should also be considered when assessing the Range of Applicability. For the higher SMLs, this assessment should be updated for all intended use cases as more rigorous data and analyses become available. More explicitly, the ranges of applicability include: the model incorporates the necessary physics, the range of parameters and their interactions have been defined, the use cases have been validated, and UQ has been carried out. Table 7.4 provides a progressively tiered assessment of the rigors in Range of Applicability.

Table 7.4 Range of Applicability SML Descriptions

Maturity Level	Description
1	Range of applicability of the physics and data-based models are defined to satisfy the intended application.
2	All input parameter ranges and the effects of their interactions specified to satisfy the intended range of applicability.
3	Limitations implemented to control use or warn user if inputs & outputs are outside of range. Sub-model outputs generated and assessed over required ranges.
4	Models, sub-models, and their interfaces assessed for all intended input ranges and use cases.
5	Full range of applicability updated for all intended use cases.

7.4. Supporting Data (Column E)

The term *supporting data* is broadly defined here as any information utilized either as an input by a model or in the process of establishing the predictive performance of the model.

Both physics-based and data-driven models consume or rely on supporting data in a variety of ways. Models frequently require quantitative inputs in the form of physical properties. Additionally, training or calibration procedures consume supporting data to determine appropriate values of hyper-parameters or model parameters that cannot otherwise be determined by some practical measurement procedure. The verification process entails comparison of model response under carefully defined scenarios that have well-defined outcomes, a form of supporting data. The validation process requires supporting data in the form of a description of system response as determined by an empirical measurement procedure. Finally, parsing the discrepancy between empirical and model-response into input uncertainty, model error, and numerical error in the process of UQ also requires supporting data.

Supporting data must be carefully documented and archived to ensure they are available to an appropriate audience for inspection. These data need to be accessed and inspected for myriad reasons, including: substantiating claims surrounding validation, determining if a potential model use-case falls within the range of model applicability, and informing future supporting data development efforts. These uses of supporting data span the modeling tool lifecycle, and therefore a carefully considered and robust archival approach is highly desirable.

The FAIR principles describe best practices to address good data stewardship, ensuring archived data are *Findable*, *Accessible*, *Interoperable*, and *Reusable* [14,15]. We note that *Accessible* data is not synonymous with *open* or publicly available data, a common misconception. Rather, *Accessible* in this context refers to the use of standardized communication protocols (e.g., http, ftp) that can include authorization and authentication steps to ensure data access is limited to appropriate parties. Table 7.5 provides a progressively tiered assessment of the rigors in Supporting Data.

Table 7.5 Supporting Data SML Descriptions

Maturity Level	Description
1	Supporting data requirements identified and documented in coordination with Verification, Range, UQ, Validation, and Risk tasks.
2	Some supporting data available. Data documentation and archival plan developed. Access control and authentication plan in place for cases where broad accessibility is not feasible. FAIR principles considered.
3	Supporting data adequate to perform SML 3 Validation and UQ tasks over a limited range of application. All supporting data identified, documented, and archived.
4	Supporting data adequate to perform SML 4 Validation and UQ tasks for several relevant use cases. All supporting data identified, documented, and archived.
5	Supporting data documentation and archive maintenance performed as additional experience from SML 5 Validation or UQ tasks becomes available.

7.5. Model Verification (Column F)

Verification is the process of ensuring that the intended computational model is solved correctly and accurately for a given problem. By naming this category *Model Verification*, it is emphasized that verification includes the simulation software code itself and also the code in the context of a specific system of interest, including mathematical model, geometry, boundary and initial conditions, problem parameters, discretization, and numerical solution choices. Here we focus on verification for physics-based models. As discussed in Section 6, the term *verification* is typically not used for data-driven models. See that section for further elaboration on *verification* and *validation* definitions and approaches for machine learning models.

Following Oberkampf et al. [181], model verification is divided into two separate efforts: *code* verification and *solution* verification. Code verification includes (1) the numerical accuracy with which the simulation software algorithms represent the underlying model equations, (2) the correctness of the source code, and (3) simulation software quality attributes including version control and regression testing. For software that uses a discretization in space or time to solve ordinary or partial differential equations, calculation of the rate of convergence toward a known analytical solution with grid or timestep size refinement for a test problem is an example of code verification, because even small coding errors may affect the observed rate of convergence [182]. Code verification is primarily the responsibility of the simulation software developer.

Solution verification refers to the determination of how accurately the discretized model computes QOIs for a given system. Unlike code verification, solution verification is usually performed for problems without analytical solutions. Use of a technique such as Richardson extrapolation [183] to establish that discretization error is acceptably small is an example of solution verification. It is primarily the responsibility of the simulation software user or analyst.

Because code and solution verification are required for reliable simulations, it is expected that a code and model may reach a high maturity level sooner in this category than in others. For example, a Model Verification Maturity Level of at least 3 is preferred before systematic validation is performed. Table 7.6 provides a progressively tiered assessment of the rigors in Model Verification.

Table 7.6 Model Verification SML Descriptions

Maturity Level	Description
1	Code and solution verification plan developed. Preliminary and informal code verification performed. Version control strategy selected. QOIs for solution verification identified.
2	Rigorous code verification completed for individual sub-models by demonstrating theoretical order of accuracy and/or convergence rates, where applicable. Unit testing implemented for sub-models. Version control implemented, documented, and archived.
3	Rigorous code verification completed for relevant combinations of sub-models by demonstrating theoretical order of accuracy and/or convergence rates, where applicable. Refinement studies completed for problems of interest, with mesh convergence demonstrated. Regression testing implemented.
4	Numerical error, including discretization error where applicable, quantified for QOIs in problem of interest and deemed small compared with validation measurement error. Regular regression testing for one or more platforms.
5	All numerical error sources (including round-off, discretization, and iteration tolerance) are understood and quantified for QOIs. Automated and documented regression testing system implemented for all relevant platforms.

7.6. Uncertainty Quantification (Column G)

Although most AM models are generally deterministic in nature, it must be acknowledged that various input parameters (e.g., thermal conductivity, constitutive properties, etc.) have uncertainty (variation) and the incorporated physical models are approximate. As such, uncertainty in predictions exists from deterministic models; understanding this uncertainty is central to developing the confidence in model predictions.

Quantifying the sources of uncertainty is central to quantifying model confidence. Model uncertainty arises from two main sources of uncertainty. The variation in input parameters is generally irreducible (aleatory) in nature in that additional information only serves to confirm the variation. As such, the combination of the sensitivity of these parameters to the model output and their associated variation gives rise to uncertainty in the model output.

The second source of uncertainty is reducible (epistemic) and originates from approximations and incomplete knowledge/information. Idealized or coarsely discretized geometries as well as approximated physics (e.g., idealized constitutive behavior, boundary conditions) both give rise to epistemic uncertainty. While often more difficult to quantify, addressing these sources of uncertainty can be used to improve model confidence.

While most of the model UQ activities require that the model has progressed to an advanced state of maturity in its development, UQ activities are not restricted to occur only after the model has been fully developed. AM models are often complex and require multiple physics sub-elements (e.g., thermal and heat transfer, metallurgical thermodynamic state and phase change kinetics, crystal plasticity, etc.) in AM PSPP modeling. As each of these sub-elements is integrated into the overall model in a hierarchical manner, UQ should also be performed in a hierarchical manner, starting with the individual sub-elements and progressing through the overall model. Deterministic sensitivities of model parameters can be evaluated at the sub-element level and propagated through the model hierarchy. Additionally, understanding the approximations of the physics often occurs during sub-element development where the influence of the approximations is explored (e.g., the influence of geometric defeaturing, various constitutive models, boundary condition idealizations). It should be noted that UQ at the sub-model stages early in development could drive additional data requirements (e.g., data that could reduce UQ in inputs, material properties, and boundary conditions).

Table 7.7 provides a progressively tiered assessment of the rigors in modeling UQ.

Table 7.7 Uncertainty Quantification SML Descriptions

Maturity Level	Description
1	Parameters of interest and UQ plan defined.
2	Deterministic sensitivity study performed on selected input parameters to quantify influence on QOIs. One-at-a-time, DoE, and expert opinion coupled with sensitivity analysis performed for input parameters. Parameters and range of outputs identified.
3	Random variables identified and quantified. Probability-based UQ analysis performed for sub-model outputs. Probabilistic sensitivities quantified.
4	UQ analysis per SML 3 performed and documented for the QOIs from full model for all relevant use cases. Probability results available for validation for all QOIs.
5	FAIR modeling & measurement data summarized. Results compared against industry-accepted, benchmark, or standard cases as available. Results documented and reviewed for validation for all QOIs.

7.7. Model Validation (Column H)

Introducing CM into the Q&C process requires rigorous model validation. Some excellent references for validation include the ASME *Standard for Verification and Validation in Computational Solid Mechanics* [162], a corresponding ASME illustration of these concepts [171], a Sandia report on *verification, validation, and predictive capability in computations engineering and physics* [173,184], and a TMS publication, *Accelerating the Broad Implementation of Verification and Validation in Computational Models of the Mechanics of Materials and Structures* [166]. A general discussion and outline for model V&V is provided in Section 6.

The validation approaches described in these references were primarily developed for well-defined topical areas such as solid mechanics or fluid dynamics. For AM, the relevant physics spans a wide range of physical processes over broad length and time scales, such that no single modeling approach is adequate. Thus, multi-physics, and multi-scale simulations using coupled modeling approaches are required for Q&C activities. Validating such codes greatly complicates the validation process; the maturity levels found in Table 7.8 reflect this process.

For low SML, the primary requirements are to define the validation needs for the given application and to develop a corresponding validation plan for all sub-models and the full intended use case. The sub-models will typically use a single simulation method. For SML 3, all sub-models must be validated using approaches comparable to those described in the validation references. Higher SML simulations are expected to include several coupled sub-models encompassing multiple scales and physical phenomena. This coupling puts significant extra demands on the validation process, so it is recommended that the inputs and outputs of each model be separately validated. Ideally, a coupled series of validating measurements should span a single complete AM process in a seamless fashion. Such hierarchical benchmarks are described in greater detail in the validation section of Appendix III A3.6 Model Validation. The validation needs for SML 5 are similar to those for SML 4, except that the simulations must be validated over the full range of applicability.

The discussion about validation requirements for this SML framework centers around physics-based models. The requirements for validating data driven models are significantly different and it is not yet clear how to define the necessary validation metrics. Validation for data driven approaches is discussed in Section 6.5.3.

Table 7.8 Model Validation SML Descriptions

Maturity Level	Description
1	Validation requirements defined for selected application.
2	Validation plan developed for both intended use and all sub-models.
3	Sub-models validated against established benchmarks or equivalent data. Model output similarly validated for specific cases.
4	Model and sub-models validated for all relevant use cases using established hierarchical benchmarks or equivalent data.
5	Model fully validated over range of applicability using validation data, operational performance data, and experience.

7.8. Performance Risk Assessment (Column I)

Risk is defined here as a degree of uncertainty associated with an event or circumstance that could lead to an undesired outcome. To manage this uncertainty, it is recommended that the following process be utilized:

1. Identify risk items.
2. Assess likelihood and severity of these risks to negatively impact desired outcomes.
3. Develop mitigation plans that will reduce the chances of an undesired event.

Effective risk mitigation plans should reduce likelihood of occurrence and/or consequences to a level deemed acceptable for the application of CM based decisions.

As part of a CM performance risk assessment, a risk versus consequences matrix is needed for intended specific application cases. Risks from CM-based decisions and associated consequences will need to be identified. The intent of CM for Q&C activities is to provide manufacturing definitions for process control, part location-based material definitions, and guidance on testing locations for process qualification. The impact of model-based decisions for Q&C activities would require a high level of V&V and an assessment of risks and related consequences. A Risk Assessment Worksheet along with an example case, both adapted from [179], are included as a worksheet within the SML spreadsheet.

Table 7.9 provides a progressively tiered assessment of the rigors in assessing Performance Risk.

Table 7.9 Performance Risk Assessment SML Descriptions

Maturity Level	Description
1	Identify risks associated with CM use for application. Complete an initial Risk Assessment.
2	Risk assessment plan should be fully developed taking validation and UQ plans into account. Mitigation plans should also be fully developed.
3	Preliminary risk assessment conducted with input from validation and UQ analysis. Mitigation activities should be reviewed and assessed to reduce likelihood of occurrence and/or consequences to level acceptable for the application.
4	Risk for CM use assessed for application in component and process development and testing stages.
5	Risk assessed for application Q&C activities.

7.9. Documentation (Column J)

The documentation SML descriptors are shown in Table 7.10. Documentation is an essential aspect in the informed use of computational methods in an engineering decision-making process. Supporting documentation serves a wide range of purposes from simply describing a tool and its appropriate use through substantiating the degree of confidence to be expected from a computational output. Additionally, documentation is a key means to substantiate SML claims. Finally, generation and maintenance of documentation can be time consuming and therefore costly, so understanding requirements and appropriately budgeting for these activities is critical.

The breadth of interrelated activities and the number of parties involved in the execution of tasks described in the SML assessment framework can be considerable. The focus of the Documentation tasks at SML 1 and 2 is on the definition and description of interactions and coupling between model components, as well as planning activities defined in most of the other SML categories including: Supporting Data, Model Verification, Range of Model Applicability, Uncertainty Quantification, and Validation. Early and thorough documentation of these details fosters communication across the stakeholders and informs future work.

All models require some form of input data, and the quality and reliability of model output is affected by this input. Therefore, documenting the pedigree of these data is an important task. Increases in SML are enabled by increases in the scope of both verification and validation activities, and these in turn often rely on additional supporting data. Maintenance of the data documentation is therefore a recurring task. Note that data documentation tasks also include descriptions of how and by whom supporting data may be accessed.

Code verification tasks executed by model developers or simulation software vendors are some of the first steps in ensuring correctness in the output of a computational tool. Transparent documentation of these activities builds trust and confidence with model practitioners, ensures that expensive solution V&V activities are not initiated prematurely, and assists in configuration control activities for use in engineering practice. Solution verification tasks handled by model practitioners often require knowledge of the underlying mathematical models and the methods implemented to find numerical solutions [185].

Even well-designed capabilities previously validated on relevant benchmark problems can be misused if users are uninformed about their details. User-guides are necessary not only to inform practitioners about both the practical details of simulation software use (e.g., settings and options, file formats) but also strategic issues including known model pathologies, limits of applicability, and robustness issues. Development and updating of a functional user guide span across the SML stages.

Finally, documentation may be necessary to show compliance with requirements or standards levied by regulatory authorities [186–188]. An early understanding of the necessary documentation can streamline documentation tasks, avoiding re-work and helping stakeholders understand the value-proposition and budget for the expense of documentation related tasks.

There are many documentation tasks in each SML stage, so an activity tracking document adapted from Ref. [179] is provided in Appendix IV and as a workbook in the SML spreadsheet. This tool provides a means to track progress of the many documentation activities across all development stages and should be customized for a given application.

Table 7.10 Documentation SML Descriptions

Maturity Level	Description
1	Outcomes of SML level 1 planning and description activities for other SML criteria documented.
2	User guide initiated, SML 1 plans updated, and SML 2 activities documented.
3	User guide developed and documented. Licensing and support strategy considered, if applicable. SML 3 activities documented.
4	User guide updated to reference supporting data, UQ analysis, V&V cases. Licensing and support implemented, if applicable. SML 4 activities documented.
5	User guide updated. SML 5 activities documented.

Section 8 Technology Maturation Path

8.1. Introduction

The eventual implementation of CM tools in Q&C of future AM products and processes will require mature software with broad applicability across different material systems. Within aviation, including FAA, DOD, NASA, and other government agencies, qualification pathways are based on the ability of these technologies to reach applicable TRLs and MRLs. These metrics are widely used for the development of prototypes and physical manufacturing of non-AM products and processes. For a process or product to be qualified for application, a TRL 8 or TRL 9 determination is typically required. At these TRLs, an actual system is successfully tested in an operational environment. For NASA TRL definitions, see Ref. [189]. Concerning the material itself, there is now a system of MMLs [Rollett et al. 2025 – full citation provided as a footnote on page 2] that codifies the progression from a theoretical concept through testing, documentation and scale-up in sample size and quantities to the point where a new material is a trusted design element. Although materials development can start with the potential for a significantly enhanced property, an application must be identified so that a set of requirements and properties is defined and tested. This construct builds on similar efforts to systematize SMLs described in the previous chapter.

These metrics are less developed, however, for defining the readiness level of CM tools. In most cases, digital tools will be used to support process and product development and qualification activities for components and systems. In this support activity, the tools can be used to support or even replace expensive and time-consuming testing and characterization. Another important distinction to be made is between CM tools to be used for development of a rigorous Qualified Materials Process [2] versus those that will aid with the Q&C process for a specific part. Both applications are important, and the former may be able to employ CM tools at a lower level of software readiness when combined with targeted materials testing.

While there are many aspects of CM tools and technologies that are in need of maturation, only some of those, i.e., the ones relevant to the stakeholders within the scope of this study, are targeted here. While perhaps the most critical issues underlying the adoption of CM tools in Q&C include those of acceptance, adoption, and culture change, the technological and engineering drivers include:

- Predict process-microstructure relationships.
- Predict microstructure-property relationships.
- Predict microstructure-performance relationships (e.g., the connections between microstructure and performance metrics such as fatigue life and creep), including critical considerations like surface finish, surface particles, flaws/defects, complex loading histories, and environmental and temperature conditions.
- Avoid/control residual stress and distortion.
- Achieve build reproducibility.

- Develop and deploy NDE, including for process development, process qualification, manufacturing, quality assurance, and in-service performance.
- Quantitatively assess performance uncertainty and reliability.
- Gain regulatory acceptance for improved materials and their manufacturing processes.

All these opportunities include multiple dependencies that serve as potential topics for CM maturation. One effective methodology for describing these dependencies is visualization using simplified Ishikawa (*fishbone*) diagrams. Such diagrams are particularly useful for identifying where fundamental research conducted at universities and government laboratories can impact engineering applications. Fishbone diagrams for Build Reproducibility (Figure 8.1), Residual Stress/Distortion (Figure 8.2), and Fatigue Performance (Figure 8.3) are included here as examples showing where improvements in CM in specific areas can positively impact important engineering concerns along the path to development of a robust capability for CM-informed Q&C. These diagrams are neither exhaustive nor unique and should be considered as examples of how the various factors can be grouped.

8.2. Build Reproducibility

Build reproducibility is a key criterion for producing affordable AM parts that meet the demanding requirements for critical applications. For a given alloy, component design, and set of application-specific requirements, build reproducibility includes factors such as the distribution of build defects, prevention and detection of build failures, local residual stresses, deleterious microstructural features after post-build processing, surface roughness, composition including selective evaporation, and powder reuse. For production of multiple components, additional factors become critical, including build variations at different parts of the build plate, variations within a single machine over time, and variations between different machines, feed stock variations, and software versions. Achieving high measures of build reproducibility between build machines with different hardware designs is particularly challenging.

Figure 8.1 is a fishbone diagram showing many of the primary inputs and dependencies that contribute to build reproducibility, along with indications of where CM approaches (red boxes) could be utilized to improve reproducibility. The primary branches include “Process Variables,” “Process Control,” “Build Defects,” Machine Variability,” and “Alloy Design.” As mentioned previously, this breakdown is neither exhaustive nor unique and should be considered an example of how the various factors impacting build reproducibility can be grouped. These branches are also not independent. For example, “Process Window” under “Process Variables” clearly affects the development of “Porosity” under “Build Defects.”

The “Process Variables” branch reflects the need for tight control over the process variables and better understanding of how these process variables affect the build reproducibility. Thus, secondary branches include all aspects of process parameter “Calibration” along with “Standards and Best Practices” for machine calibration, maintenance, and operation. The “Process Window” secondary branch reflects the need to keep the process variables within specified bounds to ensure reproducible build quality. Process modeling can play a critical role in identifying the needed process window boundaries and the degree of calibration required for a given component and application. Maintaining tight calibration can be both expensive and time consuming, requiring significant downtime for each build machine. Process modeling can be used to help determine reasonable calibration limits that balance costs and application-specific requirements of build reproducibility.

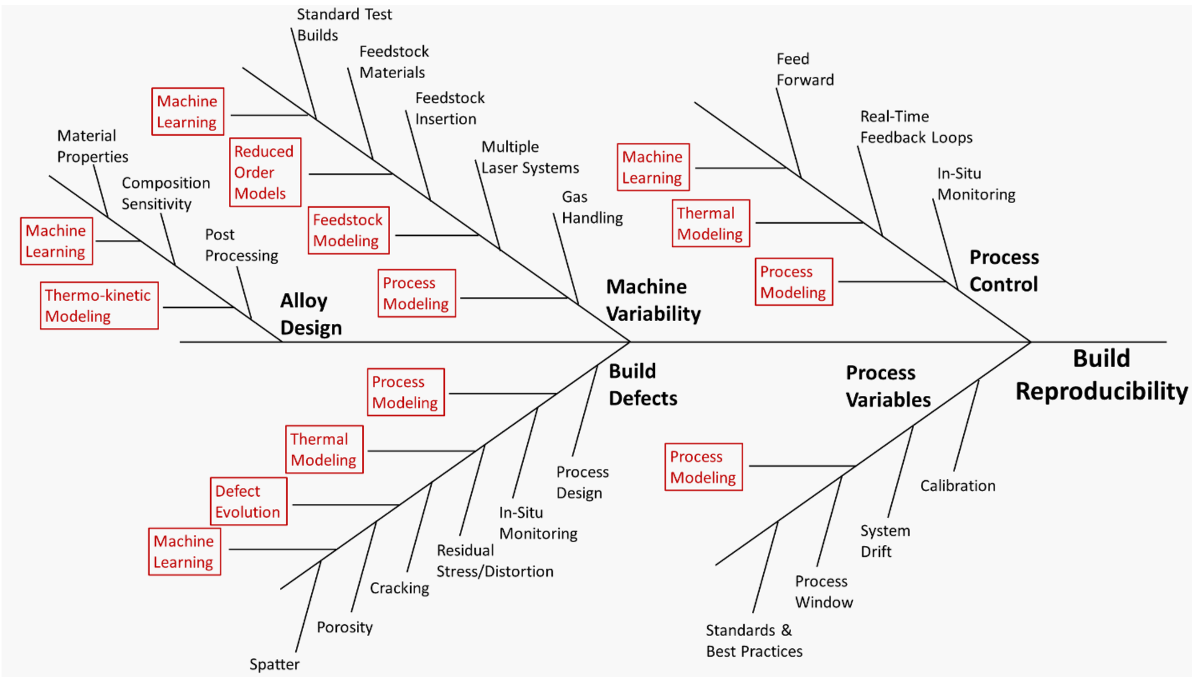


Figure 8.1 Fishbone diagram showing inputs and dependencies that contribute to build reproducibility.

The “Process Control” branch in Figure 8.1 shows connections between “In-Situ Monitoring” of the build process and process control methodologies such as “Feed Forward” design and “Real-Time Feedback Loops” that can enhance build reproducibility by dynamically varying the process parameters to adjust for local changes in part geometry and scan path. Several studies have demonstrated the importance of these approaches [190–193], and a wide range of modeling methodologies can provide critically needed understanding and inputs. Relevant modeling approaches include process modeling, multiscale simulations of the laser-powder interactions, and ML.

The “Build Defects” branch lists a variety of important defect modes that can seriously impact build reproducibility along with mitigating approaches such as “Process Design” and “In-Situ Monitoring.” Modeling can play a major role by elucidating the mechanisms and conditions for flaw formation and helping to optimize the process design and monitoring protocols. Relevant modeling approaches include process modeling, multiscale simulation of flaw formation, and ML.

Another key factor for build reproducibility is “Machine Variability.” As mentioned at the beginning of this sub-section, variability of the as-built and post-processed material can occur at different parts of the build plate, within a single machine over time, and between different machines and software versions. Sufficient levels of process parameter calibration and the use of machine-specific, real-time feedback can reduce machine variability, but complicating factors such as the local gas flow and composition, scan speed and direction, incident laser angle, and feedstock variations make it difficult to ensure that all relevant factors are sufficiently controlled. Modeling is badly needed to provide an understanding of how the various complicating factors affect the end product and to explore mitigating procedures. Relevant modeling approaches include process modeling, feedstock modeling, and ML.

The last major branch shown in Figure 8.1 is "Alloy Design" that includes developing new alloys for AM process conditions, specifying tighter composition specifications for existing alloys, and designing alloy-specific post-build heat treatments. Most alloys used for AM were developed for other processing approaches such as forging, casting, and welding. It is not surprising that only a small fraction of existing alloys is suitable for AM. Even commonly used AM alloys can introduce problems. For example, the solidification microstructure of as-built nickel alloy 625 can develop deleterious δ-phase precipitates when traditional heat treatments are applied [194], and 17-4 stainless steel built using nitrogen-atomized powder includes a large amount of unwanted retained austenite after heat treatment due to austenite stabilization by trapped nitrogen [195]. Thus, ICME alloy and heat treatment design approaches using thermo-kinetic modeling and ultimately ML are needed to improve build reproducibility for a broadened range of AM-compatible alloys. Such work is already in progress, but improvements in the thermo-kinetic modeling approaches and broader application of these techniques are needed to accelerate development of improved AM alloys and targeted heat treatments.

8.3. Residual Stress/Distortion

The cause-and-effect (fishbone) diagram in Figure 8.2 lists the variables that play a role in the residual stresses resulting from the PBF-LB AM process. Prediction of the residual stresses developed during the manufacturing process is important for at least two reasons: 1) residual stresses lead to distortion, cracking, and possible failure of the built part, and 2) residual stresses that are not relieved during the post build heat treatment process can lead to undesired effects on the performance of the part, most importantly tensile residual stresses reducing the life of the part. Residual stresses develop due to the constraints on the solidifying melt pool imposed by the relatively colder previously built layers and the interaction with the build plate. The residual stresses in the solidifying melt pool are tensile because the solidified material is prevented from contracting as it cools due to the constraint of the underlying layers. Engineering mechanics dictates that thermal stresses develop because of thermal gradients and the boundary constraints of the part/structure.

There are a large number of variables that play a role in the development of residual stresses, as outlined in Figure 8.2. The material and its properties, the part design, the process variables, and the constraints, as applied by the build plate and the supports, all play a role. Because few parts are used in the as-built state, post-build processing such as heat treatments and machining can significantly affect the distributions and magnitudes of the residual stresses. The "Uncertainty and V&V" branch is included to show that the variability of residual stresses and distortion is important for understanding possible issues with distortion variability that may affect function. In addition, it is important for the V&V of the CM tools used to perform prediction of the residual stresses.

The class of CM tools of interest here is that which predicts the residual stresses and distortion. The prediction of residual stresses is typically done via the FEA method using an eigenstrain approach. The fidelity of the solution depends partly on the discretization type and size, which can include a layer lumping approach. The thermal gradients necessary to perform such simulation are determined by the items listed in the "Process Parameters" branch. The material properties needed are listed in the "Materials" branch and the constraints are defined by the items listed in the "Build Plate" and "Supports" branches. Such lists are of course not exhaustive; for example, one could list the effect of the purge/crossflow that is part of the operating characteristics of the AM equipment.

A good description of the governing equations that describe the phenomena and processes involved in AM and residual stresses can be found in Megahed et al. [148]. A comparison of predicted residual stress against experimental measurements can be found in Watkins et al. [196]. These comparisons show that the spatial distribution of the residual stresses have the same trends but differ in magnitude. The difference may be due to the variation in the measured interatomic spacing, which is used to calculate the residual stresses for the experimental measurements, or it could be because of the discretization approach and/or the assumptions regarding the calculation of the eigenstrains. The path to maturation of residual stress/distortion prediction may simply consist of exercising the tools to elucidate the best strategies for discretization and other assumptions and improving the experimental measurement techniques such that validation can be accomplished. See Appendix V, Example Success Stories: Computation of Residual Stress, for further information on residual stress simulations for both aviation and AM.

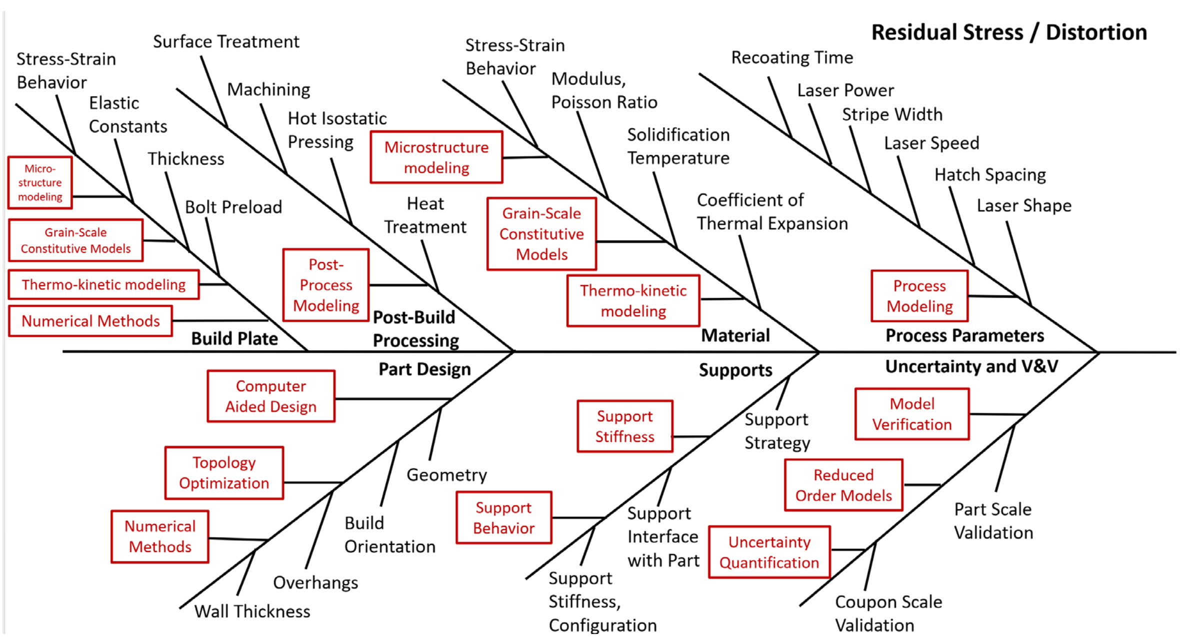


Figure 8.2 Fishbone diagram showing inputs and dependencies that contribute to Residual Stress/Distortion.

8.4. Fatigue Performance

Consistent, repeatable performance under fatigue loading is a key factor considered during Q&C. Fatigue is a weakest link problem where cracks often initiate at surface features, processing flaws or microstructure anomalies. Some initiated cracks do not lead to failure whereas others do, as governed by the local microstructure and stress state, until they reach a size where the crack front samples so many grains that a homogenized (averaged) behavior can be assumed. Once the crack becomes sufficiently large, fatigue crack growth is well-described by concepts of continuum fracture mechanics including the Paris Law.

Figure 8.3 is a fishbone diagram showing many of the primary inputs and dependencies that contribute to fatigue performance along with indications of where CM approaches (red boxes) could have substantial impact. Factors considered in assessing fatigue performance include the Local Loading and Environments, NDE of pre-existing manufacturing and service-induced flaws, Process – Structure Relationships, Structure – Performance Relationships, and assessment of Uncertainty and V&V. In aggregate, these branches represent a path toward development of uncertainty quantified PSPP relationships leading to estimation of fatigue performance. However, again this breakdown is neither exhaustive nor unique and should be considered as an example of how the various factors impacting fatigue performance can be grouped.

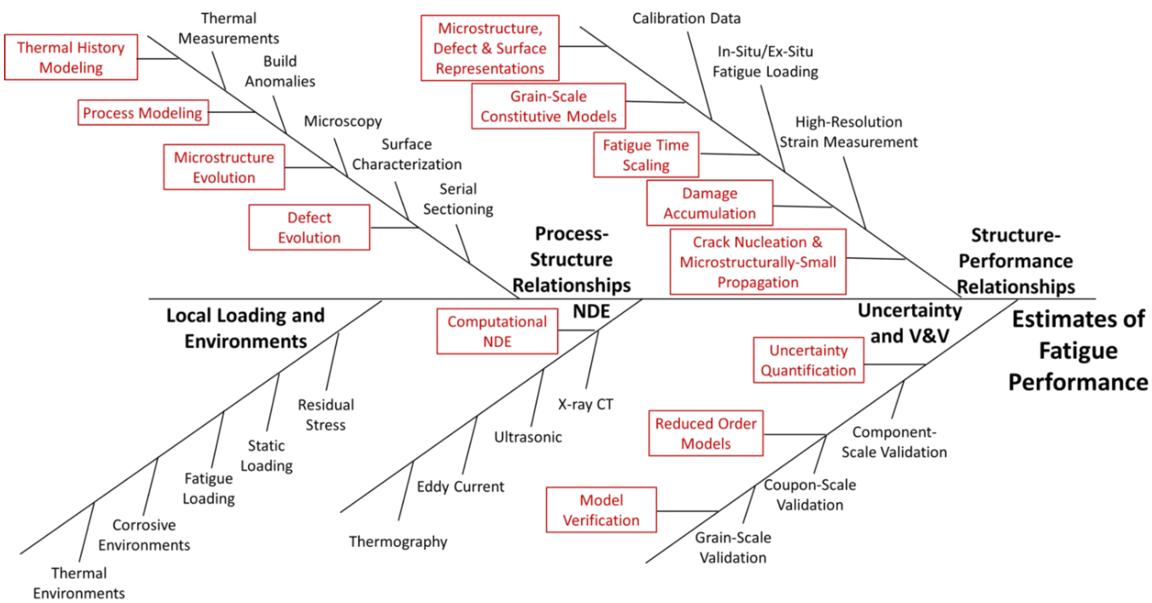


Figure 8.3 Fishbone diagram showing inputs and dependencies that contribute to Estimates of Fatigue Performance.

The Local Loading and Environments branch represents the various types of loading and environments that may result in various types of deformation and damage. The secondary branches include these various factors, including Thermal Environments that influence specific deformation and damage modes in addition to driving thermal stresses, and other environmental factors such as Corrosive Environments that degrade material properties (e.g., due to moisture or combustion products). Both Static Loading and Fatigue Loading are considered in addition to Residual Stresses that result from processing history.

The NDE branch represents some of the NDE techniques that can provide insight into the as-manufactured or in-service state of a material. Some of these techniques (e.g., ECI) are a part of the standard practice for in-service inspection while others (e.g., X-ray CT) are more applicable to the development process. Others such as Thermography and some Ultrasonic approaches are being adapted to support AM. The emerging area of Computational NDE is becoming increasingly important for designing NDE procedures and, potentially, for augmenting physical NDE.

The Process-Structure Relationships and Structure-Performance Relationships branches are often connected as PSPP relationships that ultimately describe the relationships between processing history/material thermo-physical properties and resulting mechanical properties and fatigue performance.

The Process-Structure Relationships branch includes measurements leading to an understanding of thermal history and build anomalies. Microscopy of various levels of fidelity, including optical, SEM, TEM, and synchrotron-based methods (e.g., high-energy diffraction microscopy (HEDM)) can be used to characterize flaws and microstructure. Here, X-ray CT, as previously described under the NDE branch, can also be used. Because fatigue cracks can be driven by features of as-built surfaces, Surface Characterization is also an important capability. Finally, destructive Serial Sectioning is often used in conjunction with Microscopy to complement other characterization approaches. Relevant modeling approaches span Thermal History Modeling, Process Modeling, and both Microstructure Evolution and Defect Evolution modeling with the goal of predicting the location-specific as-manufactured state.

The Structure-Performance Relationships branch includes development of the calibration and validation data needed to support model development in this branch. Some of these data must be developed using in-situ (e.g., in SEM) testing and High-Resolution Strain Measurement (e.g., in-situ image correlation, high-resolution EBSD), while other data may be collected using more conventional ex-situ testing. Simulation begins with development of accurate representations of the Microstructure, Defect, and Surface Representations and use experimental and modeling outcomes from the Process-Structure Relationships branch as a starting point. Relevant modeling approaches include grain-scale constitutive models, implemented within an FEA or other numerical framework, that are often based on variants of crystal plasticity and lead to estimates of deformation and damage accumulation. These simulations must account for the underlying extreme value statistics of crack nucleation and typically employ statistical volumes of materials sampled from appropriate property distributions. Further, since explicit simulation of each fatigue cycle is computationally prohibitive, approaches for fatigue time scaling or linearization and extrapolation of deformation fields are used. If performance beyond crack nucleation is to be considered, approaches for microstructurally small fatigue crack propagation are needed.

The final branch highlighted on Figure 8.3 is the Uncertainty and V&V branch. These capabilities are needed to give confidence to the Estimates of Fatigue Performance. Validation is needed at multiple scales and leverages capabilities discussed on other branches at the grain scale, coupon scale, and component scale. Model Verification is required for all modeling approaches discussed on this fishbone diagram. Additionally, UQ, often facilitated by Reduced-Order Models, enables determination of the dependence of uncertainties in estimated fatigue performance on each of the other parameters and provides confidence in the fidelity of the predictions.

8.5. Maturation of CM Methods

Most of the CM methods described in this document require additional maturation before they can significantly impact Q&C. These include physics-based modeling approaches as well as data-driven methods. In this section, maturation is discussed at a high level. SML requirements are discussed in Section 7 and the relevant individual modeling and measurement approaches are presented in Section 9 and Section 10.

Physics-based modeling approaches have been largely focused on development of CM tools for individual AM processes. One example is the multi-physics simulation needed to reproduce and predict the development of vapor depressions (keyholes) during high-intensity laser (or electron beam) melting in which vapor recoil pressure, Marangoni flows, buoyancy forces, and other processes must be included. Another example is modeling microstructure evolution during the solidification of successive layers which requires massively parallel computing resources to simulate the accumulation of even a small number of layers. Yet another example is multiscale heat flow modeling. The computational demands and the lack of a fundamental knowledge underpinning much of these modeling frameworks place most CM tools at the lower end of the SML scale, usually falling at an SML 2 or at most an SML 3. Such low SMLs preclude their use in Q&C for the time being.

In the short term, these tools can provide a means for generating digital data that supplement experimental measurements obtained through more traditional qualification approaches. For example, as thermal prediction tools become better calibrated and are validated against new data, their output can be used as input into microstructure prediction tools, which in turn can be correlated with property and performance variations. At every step of the way, UQ is needed to complement the calibration (or training) and validation. In the long term, both physics-based and ML models can be used as the basis for more accurate simulations that provide the means to explore larger processing ranges and provide more detailed knowledge of component performance. A more comprehensive survey of techniques and assessment of the technological readiness is provided in Section 9 which contains a table of simulation methods and the steering group’s tentative (and suitably coarse-grained) assessment of readiness and scale of investment required.

Meaningful adoption of CM tools in industrial Q&C activities will require that many milestones in a variety of contexts be achieved. As mentioned previously, required advances in CM tools involve not merely stand-alone models but also hierarchical modeling sequences in which a property prediction depends on a chain or cascade of simulation inputs. In addition to technical advances, substantial improvements are needed in ease-of-use of available simulation codes, availability of large sets of validation data, and workflows that can accommodate new sources and formats of data. Further, changes to industry's existing strategies for testing/characterization to include computational data and CM methods will be required along with *cultural* acceptance (by industry and regulatory agencies) of simulated *data* as complementary and beneficial to conventional testing and characterization approaches. In this section, we have been concerned primarily with outlining the path to sufficient maturation of the relevant simulation tools, testing methods, and materials characterization strategies. The other AM-ecosystem issues will be addressed in Section 10.

Adoption of CM tools in Q&C does not mean that all data needed for Q&C will be generated solely by the CM tools. Realistically, simulations can *supplement* targeted testing and reduce the iterative design-validate-repeat process used for Q&C as described in Section 3. Examples of these targeted measurements include characterization of the phases and precipitates in the AM-processed materials to validate the microstructure predicted by computer simulations, and location-specific mechanical testing to calibrate the mechanical models. Once calibration is accomplished, a more extensive simulation could be performed at a specific condition, and additional testing can be used to compare variability predictions. Lastly, simulations can be performed to predict properties at specific conditions of interest that may be needed for preliminary design evaluations, not only allowing the design to proceed but also defining the test conditions needed to generate the data required for Q&C.

8.6. Mechanisms for Assuring Availability of Mature Software Tools

Clearly CM relies heavily on having mature sets of computational materials tools, where the SML of a given simulation can be assessed using the maturity assessment framework presented in Section 7. However, maturity of a given software tool is not the only requirement for successful adoption within Q&C activities. The software must also be available for use and be supported in the long term for continued and reliable deployment. For this purpose, there are a variety of models that may be followed to enable access to a given software tool. Successful adoption of a given code necessitates that some strategy for distribution be adopted. Several examples are described here, each of which has advantages and disadvantages.

The most common deployment is via commercial off-the-shelf (COTS) codes, in which a commercial entity owns the codebase and grants access through a software license. This approach is common and accepted, having the advantage of providing a revenue stream for continued software development and support. Competition between software companies helps to drive new innovations and attractive licensing options. However, the codes in this case are closed-source, making it challenging for users to judge the robustness of the implementation or to make improvements. Development also therefore relies solely on the software development team, and improvements (e.g., incorporation of new techniques) from academic research or government laboratories are slow to occur. Because COTS codes are so heavily used by industry, new approaches are needed to accelerate the integration of academic- and government-developed software capabilities.

On the other end of the spectrum are free open-source (FOS) codes. In this case, codes are distributed publicly and freely. Anyone may view the source code, and potential changes and improvements may be proposed by anyone in the community (although there is frequently a manager of the repository who must review and approve changes). The advantages of this approach are that it maximizes availability with essentially no restrictions (depending on the specific open-source license chosen), and that innovation and improvements may broadly come from anywhere in the community of users and developers. Additionally, because of complete transparency of the source code, the implementation of any given functionality may be reviewed and verified as appropriate. Codes may also be readily customized to the needs of a specific user. The largest disadvantage of this approach is that continued development and support relies on an active user and developer community, who essentially act as volunteers. Such codes are thus vulnerable to abandoned development, without obvious recourse from interested users other than to take development responsibilities upon themselves.

Between these two extremes are government off-the-shelf (GOTS) codes. These codes are deemed to be of national importance by the government, with associated continuous funds allocated for development and maintenance. Such tools may be developed and maintained by individual institutions or through a consortium model. In many cases, these codes are open-source but may also have restrictions on distribution depending on their application. This model is attractive because long term support is guaranteed as long as usage is prioritized by the government, and in most cases, the source code is available for review and customization. However, the development and continued availability of such codes is driven primarily by government needs rather than by commercial interests.

Finally, it is possible to couple full open-source availability with commercial development and maintenance. This commercial open-source (COS) paradigm relies on a publicly available code base, but with primary responsibility for development falling on a commercial organization. In this case, commercial entities may fund the relevant organization for specific development tasks, technical support, or for general long-term maintenance. This model strikes a balance between general availability and transactional guarantees for support. The open-source nature of the code can help to foster an active user base, while avenues for commercial investment can prevent codes from being abandoned such as is possible in the FOS model. The largest challenge in this case is that of establishing a business model for the commercial organization that is self-sustaining without relying on regularly charging fees for software licensing.

8.7. Gaps

Lastly, it is useful to list current gaps that limit both CM maturation and adoption of CM for Q&C applications. These gaps include, but are not limited to:

- Acceptance by industry (beyond R&D) and regulatory agencies
    - This will involve a paradigm shift in the direction of design-by-analysis, which may be challenging for some organizations. Progress in this direction will need to be incremental with rigorous validation testing.
    - Trust in models is key along with clear business cases.
- CM tools that can robustly predict the structure, properties, and performance of additively manufactured parts, which largely necessitates use of *open* systems where detailed information about build strategy is available
- Fundamental understanding of the sources of machine-to-machine variability

- Improvements to ease-of-use of software tools
    - Software tools must be easy and convenient for industry engineers to use. They will also need to be implementable on laptops or workstations.
    - Software tools that work in different time, length, and physics regimes must support non-proprietary input/output formats enabling co-simulation/coupling.
- Availability of validation measurement data
    - As discussed in Section 6, the focus of model validation measurements is distinctly different from more traditional discovery experiments and data availability is limited. Most validation data used by OEMs for Q&C is proprietary. One example of a source for publicly available AM model validation data is AM Bench [12,13].
- Availability of material property data
    - Mean values
    - Statistical distributions when appropriate
- CM tools that are applicable to multiple material types and across multiple AM platforms
- Pervasive UQ simulation tools for CM
- Resources to conduct side-by-side CM-related and conventional Q&C activities, until CM tools are widely accepted as viable in this context
- 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

Most of these gaps are discussed in more detail in the relevant sections of the roadmap.

Section 9 R&D Investment Opportunities for CM Tools

9.1. Introduction

Incorporation of CM-informed approaches for Q&C may take a variety of forms, some of which can be executed with existing toolsets. However, maximizing the CM4QC vision will require advancements in the maturity of the associated computational materials tools and experiments. The required advances in modeling and simulation are discussed in the present section whereas required advances in the corresponding experiments are described in Section 10.

The computational advancements are provided as a list of specific capabilities organized in two tables. The first table is a list of types of CM activities, grouped according to key physics and computational themes (e.g., heat flow simulation or property prediction) designed to describe the current status for each capability along with tractability of development and incorporation into Q&C practices. The second table takes the same information and re-casts it in the form of a matrix of anticipated industry need versus the perceived challenges of implementation (or deployment). The difficulty of development and implementation are both considered, as well as the availability and maturity of existing software tools.

9.2. Status

For each topic area, the availability and readiness of relevant software tools are considered and divided into three categories: *ready*, *developing*, and *ideation*. Capabilities that may be *ready* to play a role in Q&C tend to include commercially available software with accepted validation approaches and widely available supporting data. Capabilities that are *developing* may not be readily available outside of an academic context, may experience frequent improvement and changes to underlying approaches, or have sparse supporting data that may be challenging to compare against model results directly. Capabilities in the *ideation* stage may not be available in either commercial or open-source software packages and are likely undergoing early stages of development on model formulation and validation.

9.3. Tractability

Each capability is also assessed on the tractability of continued development towards deployment into Q&C practices. *Low* tractability implies cases where accepted approaches are yet to be developed, and/or require new and challenging experimental techniques for validation. *Medium* tractability indicates that accepted techniques have been developed, but are primarily limited to academic study, require maturation, and/or lack rigorous validation. *High* tractability is for simulation techniques that are readily available in commercial codes or open-source software packages, with accepted VVUQ practices judged against reliable experimental data. It is important to emphasize that each capability includes a broad range of phenomena with differing levels of modeling capabilities and tractability. Thus, the provided values are a broad-level assessment of the general field.

9.4. Key Physics Themes

CM application areas are grouped first according to key physical themes. For this purpose, the PSPP linkage formalism is used to describe tools associated with process modeling, microstructure prediction, and property/performance estimation. Note that the maturity and difficulty of development are intended to consider the challenges involved in implementing both specific physical phenomena as well as the associated computational expense. A recurring theme in this assessment is the tradeoff in these factors, with models of maximum fidelity frequently being too computationally expensive for pragmatic application to Q&C activities.

9.4.1. Process

Simulation of the thermal distribution in AM in response to process variables is valuable in its own right and is a foundation for subsequent simulations of microstructure and flaw evolution. Such models must replicate real process characteristics as closely as possible to predict the thermal conditions that drive build variability, flaw formation, microstructure evolution, etc. However, there is a significant challenge in that the relevant physics span many orders of magnitude in length and time scales, ranging from the *chamber scale* at hundreds of millimeters and hours, to the melt pool scale at hundreds of micrometers and milliseconds, and down to the solidification microstructure scales of hundreds of nanometers and microseconds. Consequently, a wide range of models exist that make tradeoffs between fidelity of the physics and the computational expense, resulting in many orders of magnitude difference in computational cost. For practical application of process modeling, different models are frequently invoked depending on the type and fidelity of output data required, either for direct usage or as input for downstream simulations. For example, simple (e.g., lumped layer) approximations to thermal history have been successfully implemented to help estimate residual stresses. In contrast, computationally intensive consideration of the liquid-gas interface, laser interactions, fluid flow, and vaporization are required for direct prediction of keyholing and spatter formation. In between these two extremes, flat surface approximations and effective heat source geometries are occasionally used to extract distributions of solidification behavior that can be used for microstructural models.

9.4.2. Microstructure

Given thermal conditions within and around the melt pool, several different approaches may be used to predict aspects of the resulting microstructure. CALPHAD and associated thermo-kinetic methods are the most mature and available. These methods may predict phase equilibria, microsegregation, and precipitation kinetics, etc.; however, these techniques are best suited for near-equilibrium conditions, which is not always a reasonable assumption for AM, and these techniques do not make predictions about many relevant features of the microstructure. For those purposes, explicit microstructure representation, such as through PF or CA simulations, provide a benefit, but at significantly increased computational cost. These simulation tools are also comparatively immature, operating primarily at an academic level. For example, CA models make a range of assumptions in their representation of microstructural kinetics, and PF models are limited to small domains (tens of µm) compared to a single melt pool, and both methods often use simplified representations of real alloy systems (e.g., only two or three chemical species). In both cases, robust calibration and validation procedures are required to increase the reliability of model predictions.

9.4.3. Properties & Performance

Given a simulated microstructure, property/performance predictions may be made based on a range of approaches from simple analytical expressions to complex crystal plasticity simulations. Again, trade-offs must be made in the fidelity of the represented physics and the computational expense of a given simulation. By necessity, the microstructure simulations and corresponding property/performance predictions can only be computed for RVEs. There is therefore a need for efficiently selecting appropriate volumes from within a component based on process dynamics. This amounts to constructing an RVE about which there is a large literature albeit with little attention paid to UQ. Additionally, the key microstructural and flaw features that dominate the properties; and, more significantly, the performance of the material will be dependent on both the alloy and process history. Accurate identification of key features for specific cases is another critical capability, along with the ability to validate that the key features are appropriately captured by upstream models and/or experimental observations. Unfortunately, properties that are comparatively easy to predict (e.g., YS) are frequently not the limiting factors for component performance. More complex property/performance sensitivities, such as fatigue life, creep rates, or environmental degradation (e.g., corrosion), are often critical parts of Q&C; however, the associated CM tools are immature, or computationally expensive, or both.

9.4.4. Calibration & Validation

All these modeling approaches are dependent on relevant and accurate calibration and validation data to an extent much greater than the now commonplace ICME. Characterization, of both the process and material, at operative length and time scales is therefore a significant need. Many existing techniques have been applied for this purpose. For example, in-situ process monitoring has become commonplace on commercial systems. Additionally, several AM powder bed surrogate systems have been installed at synchrotron beamlines for high-rate imaging of processing (e.g., dynamic X-ray radiography (DXR)) and diffraction analysis (e.g., HEDM). At a laboratory scale, post-process materials characterization using X-ray CT and conventional metallographic characterization, including serial sectioning, has also been used for the required model calibration and validation. However, several challenges remain.

Characterization is expensive and time consuming, so faster and more automated processes would benefit model predictive capability. Characterization of residual stress is also a significant challenge. Operando techniques, such as in-situ DIC or diffraction-based methods, will be important for generating more relevant datasets. Additionally, the specific datasets required for each type of model must be identified along with appropriate characterization methodologies. For calibration purposes, specific experiments should be defined that provide easily characterized, yet relevant datasets.

9.5. Key Software Themes

9.5.1. Software Infrastructure

A key need for CM infrastructure is the ability to couple multiple simulation tools and compute uncertainty distributions for the key output parameters of interest. Software tools for UQ can be of two types: intrinsic within the physics simulation code or extrinsic to the physics simulation code. Typically, commercial physics-based simulation codes do not include intrinsic modules for UQ. Where available, modules are limited to Monte Carlo sampling, which is generally not computationally affordable for complex simulations. Although extrinsic tools are suitable for many applications (e.g., surrogate model fitting), there are some approaches that are only possible with intrinsic tools. For example, some academic physics simulation codes have automatic differentiation capability, a trend that has become more common with the development of libraries such as Sacado and JAX [197,198]. This approach can be used to compute first- or second-order approximations of the variance of the model output that can then be used for sensitivity analysis. The *a posteriori* error estimation capabilities in some codes are useful in model verification. These are forward UQ capabilities; none of the current physics simulation codes have inverse UQ capabilities (i.e., model calibration).

Extrinsic UQ tools can be combined with physics simulation software to perform both forward and inverse UQ in an affordable manner using surrogate models or probabilistic analysis methods that are far more efficient than Monte Carlo. In a typical implementation, the UQ tool calls the physics simulation code multiple times to develop the input-output data. These data are commonly used to build a regression-based surrogate model of the physics simulation code, which can then be used for forward prediction UQ as well as physics model calibration, i.e., estimation of physics model parameters (inverse UQ). Some commercial software [199] has the capability for DoE to decide the settings for the physics simulations. The input-output data can also be used with many open-source machine learning tools available to build advanced surrogate models. Open-source software modules for sensitivity analysis, advanced surrogate model building, and Bayesian model calibration are also available, for example, UQLab [200], UQPy [201], OpenTURNS [202], TASMANIAN [203], and Dakota [204]. All such tools require the engineer to develop the interface between the physics simulation code and the desired UQ module.

Publicly available software for uncertainty aggregation does not currently exist, whether it is the aggregation of various model errors or the aggregation of aleatoric and epistemic uncertainties. The methods, based on Bayesian networks and auxiliary variable approach respectively, have been developed [205,206], but only reside in academic research codes. These methods also aggregate the results of model V&V towards prediction UQ.

Computation of *tail* behavior (e.g., 1/1000 event or smaller) requires an inordinate number of computations for standard Monte Carlo methods. Quantification of these rare events requires a dedicated and focused UQ method. In this case, typically a small *important* region of the random variable space dominates the computation. Importance sampling (IS) is a UQ method whereby the important region is identified using a small number of samples yielding high efficiency compared to standard Monte Carlo. The effort to identify the important region is problem specific although some general IS algorithms are becoming available. More research to develop methods specific for CM models and AM are required.

The ability to compute high-quality partial derivatives of computational materials models, particularly of AM processes, will provide crucial information towards the understanding and optimization of computational models to support Q&C processes [207]. The sensitivities will be useful for a myriad of tasks such as parameter ranking, inverse problems, model calibration, reduced-order models, fast approximations for UQ, and allocation of experimental efforts, among others. This information will be particularly significant for models of the AM process due to the large number of parameters. New methods of automatic differentiation, both intrusive and nonintrusive, are required such that existing high-fidelity models can be easily enhanced to also compute sensitivities [208,209].

9.5.2. Accelerated Computation

In almost all applications of computational models, there is a tradeoff between model fidelity and computational expense. Frequently, the expense of models limits their application to a limited set of representative cases or forces the user to neglect certain physics based on assumptions about the problem at hand. For example, Figure 9.1 shows a comparison between three common types of melt pool-scale models that include different physical fidelity, ranging from a simplified semi-analytical heat conduction code to a full-physics model that incorporates effects of vaporization and liquid-vapor surface deformation. The computational cost of these models spans almost nine orders of magnitude. Consequently, to accurately and efficiently represent the process at an appropriate scale, it will be necessary to balance these tradeoffs, or combine multiple types of models, to rapidly compute an accurate estimation of thermal conditions that drive subsequent quantities of interest (e.g., residual stress, microstructure).

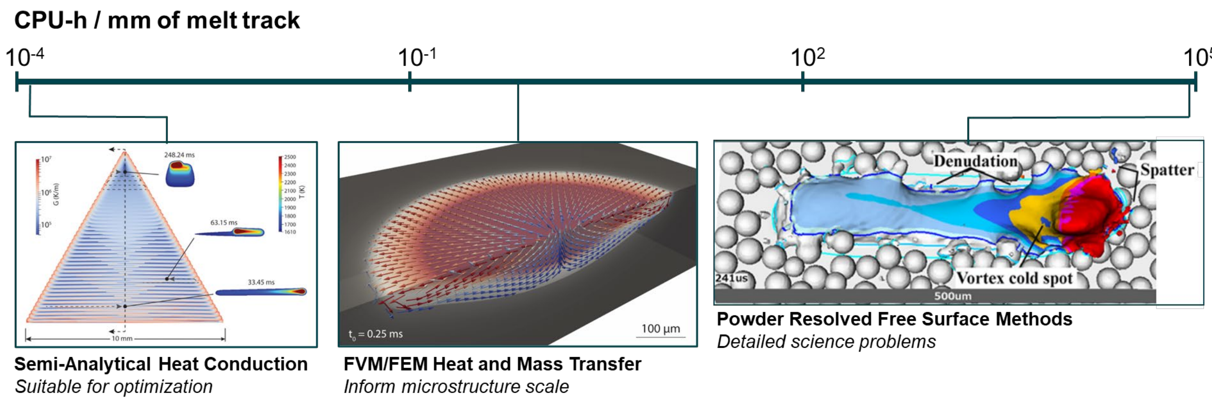


Figure 9.1 Comparison of computational expense for melt pool models at different physical fidelities [210]. Here, the acronyms are finite volume modeling (FVM) and finite element modeling (FEM).

Although Figure 9.1 uses thermal modeling as an example, similar tradeoffs between computational expense and physical fidelity are present for most aspects of AM simulation. For example, prediction of residual stress and distortion is a focus of several existing software tools. These simulations are, by necessity, performed at the component scale, and therefore, they often require simplifications to the thermal field and the constitutive material behavior (i.e., inherent strain) to make timely engineering predictions. More complete descriptions of the process and material behavior have been shown to result in better predictions but are comparatively expensive to compute.

Several techniques might help to accelerate computation to enable larger-scale simulations of relevant problems. Validated reduced-order, or surrogate, models that predict the macroscopically required quantities (e.g., residual stress, spatter potential, and thermal history) may be used on their own or to enable UQ. Additionally, large quantities of process, characterization and testing data are expected to be available through the course of the Q&C process. The emergence of AI and ML techniques may offer an approach to utilize these data to accelerate simulations of the performance of components or identify specific flaws or material metrics using processing data. Meshing these data with physics-based modeling predictions may be a viable approach to improving component performance predictions. Analyzing data from multiple data streams, including both experiment and simulation, is, however, a significant challenge and may require development of AI tools to take advantage of all available information.

A promising recent accelerated UQ method is the development of multi-fidelity sampling whereby sampling is carried out using an ensemble of models of varying fidelity and efficiency [211]. Multi-fidelity sampling works by combining the efficiency of low-fidelity models and the accuracy of high-fidelity models to provide a method with fast convergence using only a limited number of high-fidelity simulations. This approach requires the development of correlated multi-fidelity CM models. The high-fidelity model provides high accuracy of the QOIs but the computational cost is high, thus preventing the use of standard Monte Carlo sampling. The low-fidelity model(s) are constructed using simplified physics and/or a coarser discretization but capture the *essence* of the underlying problem.

9.6. Summary of Research Needs for CM Tools

In Table 9.1, each line mentions a CM application area and gives a qualitative assessment of the status of related tools and the tractability of further maturation. Comments have been included in Appendix VI to justify the rating and provide examples of R&D investment that might lead to increased maturation. The intention of this table is to give a sense, at a glance, of the status and tractability for maturation of key research areas of direct interest to Q&C practices. Areas within the table are grouped according to key physics and software themes. The status and tractability for each capability is given a grade according to the assessment of the CM4QC steering group.

This grading system is meant to help researchers and funding agencies target Q&C-relevant development activities that are consistent with their expertise and interests. For example, CALPHAD models (using well-assessed databases) are generally considered to be relatively mature, with established pathways for further development. Therefore, R&D investment may be targeted towards specific Q&C applications, rather than fundamental tool development with respect to CALPHAD techniques. R&D projects in this space therefore are likely to interest commercial software vendors, aviation OEMs, and regulatory agencies. On the other hand, *environment effects*, while highly important for aviation applications, are poorly understood for

AM materials, with few if any available toolsets for prediction. R&D opportunities may therefore focus on fundamental development and assessment of new tools that relate processing, composition, and microstructure to corrosion and other long-term environmental concerns. Investment in this case will likely include government and academic organizations interested in low-TRL efforts. While it is not within the scope of this document to detail every possible research activity relevant to the future of Q&C practices, an abbreviated explanation and examples of investment opportunities are provided in Appendix VI.

Table 9.2 gives some specific examples of opportunities for R&D investment based upon the relative timeframe anticipated for implementation (near, mid, and long term) and the level of challenge of implementation and incorporation into Q&C activities. The purpose of this table is to provide only a snapshot of possible opportunities and is not designed to be exhaustive of all possible investment areas that might be derived from the range of tools listed in Table 9.1.

Table 9.1 Status and tractability of CM tool development with respect to Q&C needs.

Thematic Area	Topic	Status	Tractability
		Ideation	Low
		Developing	Medium
		Ready	High
Physics: Process	1. LOF porosity [89]	Developing	High
	2. Residual stress [57]	Ready	Medium
	3. Distortion [57]	Developing	Medium
	4. Full-part thermal history [212,213]	Developing	Medium
	5. Build-chamber-scale effects (thermal history/gas flow, etc.)	Developing	Medium
	6. Keyhole and entrapped gas porosity [79]	Developing	Low
	7. Spatter prediction and induced flaws	Ideation	Low
	8. Melt pool dynamics (e.g., fluid flow, keyholing) [214,215]	Developing	Low
	9. Solidification conditions [214]	Developing	Low
	10. Melt pool variability	Ideation	Low
	11. Gas flow, plume, and laser interactions [216]	Ideation	Low
	12. Powder flow and effects [217]	Ready	Medium
	13. Powder recycling	Ideation	Low
	14. Dissolved gas porosity [218]	Developing	Low
	15. Surface roughness [219]	Ideation	Low
Physics: Microstructure	16. Computational thermodynamics [220]	Ready	High
	17. Thermo-kinetics	Ready	Medium
	18. Grain-scale microstructure [110,221,222]	Developing	Low
	19. Sub-grain microstructure [223,224]	Developing	Medium
	20. Dislocation structure	Ideation	Low
	21. In-process cracking [225]	Developing	Low

Table 9.1 continued. Status and tractability of CM tool development with respect to Q&C needs.

	Topic	Status	Tractability
Physics: Properties and Performance	22. Static mechanical properties (YS, work hardening) [226]		
	23. Static mechanical properties (ductility, ultimate tensile strength (UTS))		
	24. Creep		
	25. Fatigue life (initiation and short crack growth) [227–233]		
	26. Fatigue life (long crack growth) [234,235]		
	27. Fracture toughness		
	28. Environmental effects		
	29. Part scale geometric effects [236]		
Software: infrastructure	30. Non-intrusive UQ [203,204]		
	31. Intrusive UQ		
	32. Model validation		
	33. Model coupling infrastructure		
Software: Accelerated Computation	34. Machine learning/surrogate models [237]		
	35. Physics-based reduced-order models		
	36. Hybrid ML/Physics-based models		

Table 9.2 Matrix of industry need versus implementation challenge.

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) • Flaw 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 • Flaw prediction: keyhole porosity via ML • Distortion from thermal contraction • CALPHAD Sheil calculations for solidification • Thermokinetics: kinetics of precipitation (TTT, CCT) [*where diffusion data is not available, or for highly heterogenous 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 simulation or hybrid CFD-FEA approach • Flaw prediction: keyhole, LOF, or stochastic porosity via full-field fluid flow simulation or hybrid CFD-FEA approach
Strong Benefit/Need	• Flaw 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/performance: 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 and 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

9.7. Suggested Research Approach by Timeline

The different levels of maturity and challenges associated with development for each tool implies a difference in both the timeline for development and implementation, as well as the stakeholders most likely to be engaged for that purpose. Broadly, an appropriate approach in a particular case may be qualitatively classified by the time horizon anticipated for Q&C adoption.

Near-term (1-5 years):
In the near-term, it will be necessary to identify approaches to incorporate existing commercial software to help guide Q&C activities, such as designing experiments or guiding testing practices, even if they are not directly incorporated into Q&C requirements. In this case, partnerships between commercial aviation organizations and commercial software vendors should help to identify and execute specific work scope based on the industrial needs. For example, where a (commercial) code exists but validation data from which UQ can be developed does not yet exist (best of all in a publicly available forum), this could be a candidate for a short-term investment by the aviation industry for incorporation into Q&C practices. In certain instances, users may be willing to test (validate) research codes. Investment in these cases may come from internal funds with anticipated near-term ROI, or from industry led consortia that leverage pre-competitive government funds.

Mid-term (5-10 years):
Mid-term research will require investment of government R&D funds and should incorporate partnerships between aviation organizations, software vendors, government laboratories, and universities. The research will target emerging techniques for CM, accelerate their incorporation into commercial tools and Q&C practices, and help to develop process-aware design allowables. Doing so will require support from manufacturers and regulators to identify the most critical areas of research that are likely to have a large impact on accelerating Q&C. Funding agencies will likely need to incorporate input from both industry and academia to identify appropriate topics for funding calls.

Long-term (10+ years):
In the long-term, it will be necessary to develop new CM techniques that dramatically expand the capabilities of computational materials tools and their application to Q&C. This research might involve expanding the physical fidelity and accuracy of models but should also focus on dramatic reduction in computational expense, maximizing the Q&C value of simulations through careful optimization by computing the most critical model outputs, direct incorporation of computationally efficient UQ techniques, and adoption of data driven AI/ML approaches. Ongoing improvements in performance at all scales from laptop to supercomputer, especially via incorporation of GPUs, should be exploited. This research is best suited for government laboratories and universities with a focus on capability development rather than producing data for a specific application. However, identification of specific research topics should be prioritized based on those that target a specific connection to accelerating Q&C practices.

Section 10 CM Ecosystem Maturation Path

10.1. Introduction

A review of the current status of computational materials tools for aiding Q&C of AM components has revealed a number of shortcomings. First, the physical phenomena that govern AM processes, microstructure evolution, and relevant properties are exceedingly complex. No end-to-end solution currently exists that is capable of producing results that can be trusted for use as part of Q&C. Aside from the need to mature the physical modeling capabilities relevant to AM production, V&V practices must be codified. In addition, although UQ techniques are available, they are not commonly built into commercial software packages. Given this current state of the art, it is understandable that CM techniques have not had a significant impact on the Q&C approaches for AM aviation components to date. However, a significant opportunity exists to dramatically accelerate Q&C practices and reduce their cost if these tools can be effectively incorporated. It is essential to create an ecosystem that enables adoption of these tools for this opportunity to be realized. This ecosystem may be summarized in several key components, each of which will require strategic partnerships among various organizations:

- Investment in CM tool development
- Transition to next-generation AM machines
- Characterization and data practices for calibration, validation, and machine learning
- CM4QC culture
- Development of AM-appropriate regulatory standards
- CM education and workforce development

10.2. Investment in CM Tool Development

As outlined in the previous section, continued development of CM tools for Q&C has many critical research needs. Properly scoping, funding, and executing these activities, however, will require an ecosystem that combines the strengths of a variety of organizations. Please see Table 9.1 for details on opportunities for research investments and their potential impact on Q&C practices.

10.3. Transition to Next-Generation AM Machines to Support CM4QC

Predicting the material quality from AM necessarily requires a detailed understanding of the process itself, which requires knowledge of the in-situ process dynamics. Unfortunately, most commercially available systems do not make the actual process dynamics available to the user. Furthermore, there are a wide variety of capabilities and data availability across various systems and manufacturers. CM approaches naturally begin with modeling the process itself, and the quality of these models and any subsequent prediction depend on the accuracy with which the models represent the process. As a result, a functional ecosystem to enable CM4QC includes AM machines that measure and make detailed information available to the users. This information must include accurate representations of process variables that are currently only vaguely defined (e.g., laser spot size, and power), a detailed description of the scan path for every build, and other process data (e.g., oxygen and gas flow sensor readings). Furthermore, the behavior of the process should be as completely characterized as possible. For example, the pattern of gas flow in the build chamber is normally unknown to a user, creating variability throughout the build chamber that is challenging to model. This points to opportunities to support studies of how gas flow control has evolved over time, both with respect to inlet/outlet vents and overall build chamber design and how this has improved part quality. Similarly, variations in laser behavior across the build chamber are currently not considered.

A data rich environment for process conditions and execution is necessary and needs to include sufficient information, such as the scan path, to define simulations that accurately reproduce real processing. Additionally, these data should be complemented by a full suite of high-quality sensors. Many systems are beginning to include optical and thermal imaging modalities, and these approaches are encouraged across the industry. In addition to machine vendor installation of such capabilities, AM machines should be designed to enable the incorporation of new and/or improved sensors as they become available.

Data formats should also enable analyses using user-defined software. Current implementation of such sensors and the quality of data produced varies widely across the industry. Some community standards should be established both for valuable sensor modalities and for best practices for data collection and storage. Evolution of these data collection modes and any corresponding standards over time should seek to satisfy experimental data needs for calibration and validation of CM4QC toolsets and approaches.

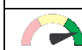
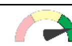
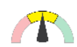
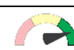
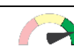
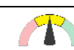
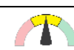
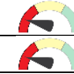
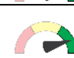
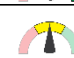
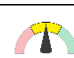
Lastly, ideal AM machines for utilization of CM4QC should be built for reliability and repeatability. If the behavior of the system is characterized to a level that successfully enables calibration and validation of relevant models, the model assessment may only need to be updated on a periodic basis. This points to opportunities to support the development of machines capable of high reliability part production in small lots, which is often the case for metals AM, for example.

10.4. Characterization & Data Practices for Calibration, Validation, & Machine Learning

As CM tools become incorporated into Q&C practices and new computational capabilities become available through additional research and software development, it is necessary to establish their accuracy and reliability through the comparison of models to benchmarks and high-pedigree datasets. Furthermore, as incorporation of AI and ML techniques becomes more widespread, there is a clear need for collection and maintenance of large datasets. Of course, individual organizations may take this task upon themselves as a competitive advantage (as is common in the aviation and other technology-focused industries) but considering the expense of collecting datasets from real-world experiments and the benefits of large quantities of data, CM4QC would benefit from pooling resources to build large, pedigreed datasets, likely requiring a government-led and coordinated effort. This will, however, require a concerted effort on the part of the materials and industrial engineering communities to build the case for long-term government support.

High-quality data are necessary for a variety of uses in a potential CM4QC framework. However, not all data are equally available, easy to collect, or low in uncertainty. Overall, we define here two categories of data, input data in Table 10.1 and output data in Table 10.2. Input data are necessary for running models. The focus here is on experimental techniques although data for some models may come from up-stream simulations. The second type of data is output data, which is used for calibration and validation of physics-based models or training of data-driven models. For each type of data, the current status of data collection is subjectively graded upon whether existing techniques are readily available and easy to use reliably. Green status indicates data that are readily and reliably collected in a laboratory setting, yellow status indicates the need for more challenging experiments, and red status designates data that necessitate experiments that are extremely difficult and non-standard. The degree of accuracy and/or precision in the resulting measurements is similarly graded qualitatively, green for accurate/precise measurements from accepted techniques, yellow for lower accuracy/precision and greater uncertainty, and red for very high uncertainty, potentially from a lack of available data. Note that parameter estimation techniques may be used as an approach for determining model inputs given experimental data for comparison to model outputs. This approach overlaps heavily with model calibration and UQ procedures as described briefly in Section 9. However well-calibrated any given model may be, a new set of data may *break* the model and require a fresh examination of uncertainty and parameter sensitivity.

Table 10.1 Input Data. The use of "(T)" specifically denotes a temperature-dependent measurement.

Thematic Area	**Data**	**Characterization Techniques**	**Current Status**  **Lab scale**  **Limited/challenging**  **Rare/highly challenging**	**Measurement Accuracy/Precision**  **High**  **Med**  **Low**
Physics - Material properties	Density	Archimedes, pycnometry		
	Coefficient of thermal expansion (T)	Dilatometry		
	Specific heat/latent heat (T)	Differential scanning calorimetry (DSC)		
	Thermal diffusivity (T)	Laser flash		
	Freezing range	DSC		
	Boiling temperature	DSC		
	Vapor Pressure	Heat pipe, Knudsen effusion		
	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		

	Data	Characterization Techniques	Current Status	Measurement Accuracy/Precision
Physics - Process (cont.)	Gas flow	Anemometer, Schlieren		
	Gas composition	Oxygen sensors, humidity sensors, etc.		
	Ambient temperature	Thermometer		
	Build plate temperature	Thermocouple		
	Powder size	Laser diffraction, microscopy, X-ray CT, sieve		
	Powder composition	Inductively coupled plasma, combustion, inert gas fusion		
Physics - Microstructure	Diffusion coefficients	Diffusion couples, isotope tracers		
	Thermo-kinetic data	Diffusion couples, electron microscopy		
	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	EBSD		
	Nucleation density solid-solid	Precipitate characterization (e.g., TEM)		
	Nucleation undercooling (distribution)	Calorimetry		
	Liquidus surfaces	DSC		
	Partition coefficients	Electron probe micro-analysis		
Physics - Properties	Dislocation density	Diffraction, microscopy		
	Grain size and texture	SEM (EBSD)		
	Precipitate size and fraction	Microscopy (SEM, TEM, APT)		
	Phase identification	Diffraction, microscopy		
	Flaw distributions	Microscopy, X-ray CT, resonance techniques		

Table 10.2 Output data.

Thematic Area	Data	Characterization Techniques	Current Status	Accuracy/Precision
Physics - Process	Melt pool size	Microscopy		
	Melt pool size	IR imaging		
	Temperature	Thermocouples		
	Temperature	IR		
	Chamber gas flow	Hot-wire		
	Distortion	Structured light		
	Post-build residual stress (macroscale, type 1)	Diffraction, mechanical release		
	In-process residual stress (macroscale, type 1)	Diffraction [238,239]		
	Post-build residual stress (microscale, type 2)	Synchrotron X-rays [238,240]		
Physics - Microstructure	Dislocation density	Diffraction, microscopy		
	Grain size and texture	SEM (EBSD)		
	Precipitate size and fraction	Microscopy (SEM, TEM, APT)		
	Phase identification	Diffraction, microscopy		
	Flaws	Microscopy, X-ray CT		
Physics - Properties/Performance	Tensile – Yield	Tensile testing		
	Tensile – UTS	Tensile testing		
	Tensile – Ductility	Tensile testing		
	Tensile – Strain hardening	Tensile testing		
	Tensile – Strain rate sensitivity	Tensile testing		
	Fracture toughness	Fracture toughness testing		
	Creep	Creep testing		
	Fatigue	Fatigue testing		
	Corrosion	Electrochemistry, salt fog		
	Thermal conductivity	Numerous methods		
	Electrical conductivity	Flash diffusivity, DSC, density		

The emergence of AI and ML techniques has created additional needs for collection of large and reliable datasets. With respect to these applications, it should be noted that existence of data does not imply suitability of those data for AI/ML training. Data must be both appropriately targeted for a given problem and collected and labeled reliably. To this end, incorporation of large datasets into development and application of Q&C tools faces additional changes. First, there is not currently a standard for establishing the pedigree and necessary context for a specific dataset. While examples are available in the tech world of establishing such practices, known as “Datasheets for Datasets” [241], nearly as soon as such standards were proposed, they were being adapted to specific use cases [242]. It will be necessary to build on these experiences to establish a “Datasheet for Manufacturing Datasets.”

In addition, hosting and maintaining data is a non-trivial task. Either an existing organization must take this responsibility (federally funded or otherwise separated from profit-driven Q&C activities) or a new organization will need to be established. In either case, the expense is likely to be significant, so a consortium of partners that share in the cost is the most likely scenario. There also needs to be incentive to contribute datasets. For example, this may be a requirement for accessing the overall database.

10.5. CM4QC Culture

One of the largest barriers to rapid adoption of CM tools for Q&C is that current approaches simply do not have procedures for making use of CM results. The naive expectation is that CM predictions may directly replace testing data. However, given the significant complexity of AM processing and resulting materials, this expectation for near-term impact is unreasonable. Instead, it is necessary to build a culture in which CM tools are frequently used to guide and interpret experiments, development, and testing based on their strengths, while acknowledging their shortcomings. Such an approach can be supported through the appropriate use of UQ techniques to establish the range of applicability and certainty of model predictions and through targeted supporting experiments.

One of the key advantages of using CM tools over relying entirely on experimental data is that they explicitly incorporate the physical phenomena associated with process dynamics, microstructure evolution, material properties, and performance. As a result, not only can thoughtful application of CM approaches help to accelerate Q&C in specific instances, but over time it will help to build understanding and intuition of the underlying physical process that will aid in long-term decision making, including computational tool development and manufacturing process maturity.

Building this culture will be challenging and require innovative thinking within Q&C processes that have been established and matured over long periods of time. In addition to technical leadership, one approach to aiding in this cultural shift is to identify and mature low-risk research activities that have a high probability of success for informing Q&C decisions. The thought process for these activities should focus on ways that CM tools can augment rather than replace existing Q&C practices. For example, CM tools can:

- Increase confidence that material testing is representative of actual components, e.g., development of process-equivalent test specimens.
- Reduce the total amount of experimental testing while still building the necessary confidence in the results.
- Shift testing towards less costly and more-efficient tests by enabling reliable extrapolation.
- Improve relevance to real components with same amount of testing.
- Reduce variability to improve designs with same amount of testing.

Successful examples of these types of approaches to accelerating or enhancing Q&C will create a competitive advantage for organizations that make the greatest use of these advances. As the maturity of CM tools grows over time to be faster and more quantitatively predictive, these near-term successes will grow quickly by enabling rapid incorporation of emerging techniques. Ideally, additional acceptance will have a positive feedback effect of increasing the regularity of V&V practices, including collecting data specifically for calibration and validation purposes and increasing the drive for rapid maturation of promising CM techniques. For a more comprehensive discussion of business benefits of incorporating CM into the Q&C process, see Section 3.4. For a worked example of applying UQ to CM, see Appendix II.

10.6. Development of CM-Appropriate Regulatory Standards

As discussed in Section 4, current regulatory standards do not specifically call out accepted methods for the use of CM tools in Q&C activities. For increased use and acceptance of CM tools, it will be necessary to establish techniques and guidelines for incorporation into certification data packages. VVUQ is needed to establish a comprehensive basis for any property predicted by CM. Good agreement between the CM predictions and experimental results represents an essential element of the validation process (as discussed in Section 6 and Section 7). Best practices for building such statistical datasets should be captured in the industry standards or regulatory guidance. Ideally, these approaches will be established through demonstrated use cases driven by interested industry partners. This bottom-up approach will help define accepted methodologies that could contribute to the development of the CM4QC framework. Consequently, there is a significant need for near-term demonstrations of ways in which CM activities might accelerate Q&C. The pathfinder exercise mentioned in Section 11 is an example of such an activity.

10.7. CM Education & Workforce Development

To enable incorporation of CM tools into Q&C practices, it is critical to generate innovative ideas while simultaneously making thoughtful, pragmatic decisions. Further, engineers in industry must understand the use and limitation of CM methods within the context of Q&C. For these purposes, an educated workforce must be developed that is aware of both the strengths and shortcomings of the available modeling tools and awareness of how they may be applied to solve challenging problems related to Q&C of flight hardware. The education and workforce development efforts should provide opportunities to the practicing professional to learn and better understand how modeling and simulation could be better incorporated within their existing workflows, and the education of undergraduate and graduate students should increasingly include these and other relevant topics. Ideally, engineering and materials science curricula should seek to incorporate aspects of the following topics, roughly ordered from most basic and general to most applied and specific:

1. Basics of mathematical models, numerical methods, data analytics, and software development
2. UQ and error analysis, both for computation and experiments
3. Combining design, experiments, and modeling tools to achieve a targeted goal
4. V&V concepts, examples, and best practices
5. AM-specific courses at the undergraduate, graduate, and professional level
6. Awareness of industrial Q&C practices and requirements

Within Topic 1, programming and numerical methods are often found in some curricula (e.g., mechanical engineering); however, simulation methodologies are less frequently incorporated into others (e.g., materials science). Although mathematical models are common throughout, greater emphasis on CM topics would be valuable. Basics of structured programming are common in engineering and science, but software development is generally only found in computer science programs. Data science and machine learning techniques are already being implemented in many fields. Greater inclusion into curricula is recommended to accelerate incorporation into Q&C practices. We note that informal tutorials on a wide range of topics have proliferated to the point where many students will check such platforms as YouTube before consulting textbooks, for example.

Topic 2 is typically covered in a measurements and instrumentation course taught at the sophomore or junior level. Methods for quantifying uncertainty from numerical models are occasionally covered at the graduate level and more sophisticated methods for experimental mechanics are covered at the graduate level. It is recommended that basic concepts of UQ for numerical models be introduced at the undergraduate level.

Topic 3 requires application of multiple tools across disciplines to solve specific problems. For instance, this topic may be incorporated into undergraduate capstone projects found in many programs with an emphasis on combining both experiment and theory/modeling. This topic could also be incorporated into graduate numerical methods classes and into regular research activities.

Topic 4 discusses the concepts of V&V that should be included in curricula. V&V could be introduced at the undergraduate level with verification reviewed in a numerical methods course and validation in regular coursework against benchmark datasets or in capstone senior design courses. The practice of V&V should be formally reviewed in a graduate probability and statistics course and an experimental methods course.

Topic 5 requires the development and presentation of interdisciplinary AM-specific courses at the undergraduate, graduate, and professional levels (e.g., short courses). Suggested topics include a survey of AM methods, the printing mechanics of various AM processes, modeling of AM processes, quality control of AM processes, and PSPP relationships. Academic institutions should develop minors or certificates for AM that enhance the core curriculum with a set of AM-specific technical electives. Short courses should be presented at technical meetings and available online with continuing education credits received by attendees.

Topic 6 is more specific to the aviation industry and is unlikely to be incorporated directly into academic curricula. Instead, it suggests an emphasis on immersive experiential learning such as internships, co-operative education programs, and sponsored projects. Organizations that are not already taking part in existing programs of this kind should consider doing so, and those that are should emphasize the use of CM tools within these experiences and projects.

Section 11 Next Steps

Publication of this document is just one step in a phased approach that may include:

- Public rollout through presentations at dedicated symposia (the first CM4QC symposium was held at MS&T 2024 in Pittsburgh, PA)
- Continued engagement through invitational workshops and public symposia
- Socialization of the new approaches for Q&C throughout the aviation industry and corresponding certification authorities
    - Facilitate development of more detailed guidance for the certification process in close coordination with the appropriate regulatory agencies
- Outreach to technology-enabling organizations such as funding agencies, government research laboratories, academia, consortia, and professional societies
- Development of ideas for best practice guides and Q&C-focused standards
- Coordination of a multi-organization pathfinder (demonstration) effort to execute a single iteration of the computational and validation loops shown in Figure 3.3 for a realistic aircraft component
- Development of possible follow-on documents, such as
    - example document for SML assessments (see Section 7)
    - recommendations list (by CM4QC government members)
    - updates to current document and expansions to other manufacturing approaches and industrial segments

Although the immediate focus has been the introduction of CM approaches into Q&C processes for AM in aviation, this example is just the first of a broader target of PIM technologies and industrial sectors. Thus, AM is intended to be the first of several manufacturing approaches to incrementally incorporate CM methods into the Q&C process. The primary reasons AM was selected for this leadoff role are that Q&C approaches for AM are not yet entrenched and Q&C for AM is fundamentally difficult, thus providing a strong motivation for CM-informed Q&C. If simulations can be successfully incorporated into AM Q&C, the resulting processes and requirements can then be more easily expanded to other manufacturing domains. Another expansion in scope that can be considered is to other industrial sectors such as space exploration (e.g., in-space welding), health care (e.g., artificial joint components), civilian nuclear power, maritime transport, petroleum and natural gas components, and non-aviation defense applications.

The CM4QC membership understands that a great deal of work remains to make the vision of this document a reality, so they intend to continue working closely with the relevant stakeholder communities to achieve the broad goals described in this strategy document.

Appendix I Examples of Government-Supported CM Efforts, Initiatives, & Software Capabilities

A1.1 Examples of CM Efforts and Initiatives

The pace of government investment in both AM and CM (and related areas) has been increasing continuously during the past several years, as demonstrated by the following examples. This document capitalizes on these trends by highlighting the benefits of increasing use of CM for Q&C of PIM technologies such as AM and charting a path forward.

DARPA Accelerated Insertion of Materials (AIM) [243]

The AIM program of the early 2000's was the first large, coordinated, CM effort and was focused on using physics-based modeling to decrease the time needed for material development. Goals of the AIM included strengthening interactions between designers and materials engineers, advancing the application of CM, and integrating CM capabilities with engineering design tools.

Notable outcomes: Within one year, material behavior models were integrated sufficiently to enable the execution of statistically designed test matrices and generation of response surfaces. Within two years, the materials behavior models were fully integrated, enabling execution of several case studies. While full-scale implementation, promising over $200M system life-cycle benefits, has experienced some industrial inertia, targeted implementation of the toolsets has been used in discrete cases to speed the qualification or reduce the risk of process changes or new alloy introductions.

National Research Council Report on ICME [10]

The report was released in 2008 and was compiled by a committee consisting of twelve SMEs from industry, government, and academia with input from numerous others. It includes a *vision* for ICME, a detailed discussion of the benefits of ICME, a series of specific targeted recommendations for government and industry investment, and suggested engagement by academia and professional societies. The vision is supported by a discussion of relevant case studies, lessons learned from those studies, and technological barriers that must be overcome for the broad use of ICME. The final discussion in the report is focused on ways to overcome the corresponding cultural and organizational challenges including educational and workforce readiness.

Notable outcomes: This report was the impetus for several programs as suggested within its recommendations section. After presentation to the Office of Science and Technology Policy (OSTP) in 2009, on June 24, 2011, President Obama announced "To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call the Materials Genome Initiative." Over the next five years, Federal agencies, including the DOE and DOD, the

National Science Foundation (NSF), NIST, and NASA, invested more than $500 million in resources and infrastructure in new R&D and innovation infrastructure to anchor the use of advanced materials in existing and emerging industrial sectors in the United States. The AFRL Materials Science and Engineering Data Challenges that initiated in 2015 further implemented some of the recommendations. "With this challenge, we're hoping to demonstrate new ways to aid materials scientists and engineers to find new, promising materials compositions much more quickly, or provide new insights into complex materials behavior that has been challenging to explain by other means," said Dr. Chuck Ward, AFRL Integrated Computational Materials Science and Engineering Lead.

Materials Genome Initiative [11]

The Materials Genome Initiative (MGI) was initiated in 2011 by the Obama Administration to "to explore the vision and challenges to be overcome in harnessing the power of computing and communications technologies for rapid development and use of advanced materials." This ongoing multi-agency effort aims to improve global competitiveness by enabling discovery, development, manufacture, and deployment of advanced materials at twice the (baseline) rate and at a *fraction* of the cost. MGI released an updated strategic plan in 2021 [244] and it continues as a major CM-related thrust.

Notable Outcomes: Since 2011, the U.S. Government agencies supporting the MGI have made large investments in the Materials Innovation Infrastructure, developing the computational, experimental, and data-driven capabilities that, when tightly integrated, can rapidly accelerate the design of new materials for insertion into manufactured products. The MGI has resulted in hundreds of new R&D efforts in the U.S. and inspired other nations to follow in their footsteps. In the U.S., some high-profile efforts include the creation of four NSF Materials Innovation Platforms (MIPs), mid-scale infrastructure programs designed to accelerate advances in materials research. MIPs respond to the increasing complexity of materials research that requires close collaboration of interdisciplinary and transdisciplinary teams and access to cutting edge tools. The NSF also established the Designing Materials to Engineer and Revolutionize our Future program (DMREF), which funds dozens of major MGI-focused projects across academia at any time. NIST responded to the MGI by turning its focus to the complex problem of materials data dissemination and quality assurance, laying the foundation for data-driven materials R&D, and anticipating the increasingly widespread application of AI techniques for materials design. NIST also increased its footprint in academic research that can support the MGI through the establishment of the Chicago-based Center for Hierarchical Materials Design, a collaboration between NIST, Northwestern, University of Chicago, and Argonne National Laboratory. The DOE established the Energy Materials Network and funded numerous efforts in computational materials science and chemistry. The DOD, via the Air Force, developed the Foundational Engineering Problems (FEP) as a way of driving ICME developments, while the DOD Army Research Laboratory (ARL) established the Enterprise for Multiscale Research of Materials to enable the design of materials for future Army Systems, and the Office of Naval Research (ONR) established the Lightweight Innovations for Tomorrow (LIFT) Manufacturing

Innovation Institute for metals processing and structural design to provide lighter-weight products, systems, and vehicles.

DARPA Open Manufacturing Program [18]

This program focused on the development of computational tools for simulating the PBF-LB AM process. The goal was to accurately model the PBF-LB process, to simulate it under various normal and anomalous conditions, and to use the knowledge gained from the results to accelerate qualification. Computational tools were developed to model the powder spreading, the melting and solidification of the powder to predict the residual stresses, the microstructural evolution throughout the postprocessing heat-treatment cycle, and to predict the strength of materials. Sensors were installed in AM machines to collect data from the large extent of experiments performed during the length of the program. Data collected were used to calibrate, validate, and verify the models; and also to develop quality metrics for in-process quality assurance of AM processes.

Notable Outcomes: For the first time, a rapid probabilistic qualification framework for AM was developed and demonstrated. Extensive computational materials codes were developed, verified, and validated over the relevant process-structure-properties range. The software release for commercial purposes was launched in November 2018.

NASA Transformational Tools and Technology Project's Computational Materials-Informed Qualification and Certification of Advanced Manufacturing-Based Materials and Structures [245]

This effort (2018-2025) was focused on development of a CM-informed Q&C paradigm based on Uncertainty-Quantified Process-Microstructure-Property/Performance (UQ PSPP) relationships that link fatigue life of AM Ti-6Al-4V and nickel Alloy 718 to microstructure and flaws and, in turn, to processing parameters. Although the effort ended before this goal could be met, some notable outcomes were achieved.

<u>Notable Outcomes</u>: This work contributed to the development of many of the component capabilities required for CM-informed Q&C, including 1) an uncertainty-quantified PSPP framework that integrates the PBF-LB process to microstructure/flaw simulations and microstructure/flaw states to property/performance simulations, 2) experimental, characterization, and measurement capabilities that provide the required calibration and validation data, and 3) a well-integrated platform for prototyping computational materials-informed capabilities and understanding their potential role within the Q&C domain. The effort is envisioned to advance the rapid maturation and transition of CM R&D as the foundation for OEM-relevant Q&C engineering capabilities.

AFRL AM Modeling Challenge [246–250]

This effort was focused on improved understanding of the internal structure and resultant performance of metallic components produced by AM and consisted of four challenges used to assess the state-of-the-art in prediction of macro-scale process-to-structure, micro-scale process-to-structure, macro-scale structure-to-properties, and micro-scale structure-to-properties. AFRL has subsequently become a measurement partner under the broader NIST AM Bench effort discussed below.

Notable Outcomes: Modeling challenges concluded in 2020 and garnered 20 responses across 16 unique respondents. A general trend that emerged when comparing modeling results with measurements was that while a baseline predictive performance was achieved by most responses, top performers were distinguished by predictions in complex conditions (i.e., predictions of melt-pool geometry under transient versus steady-state behavior, grain-scale strain predictions in the elastic versus plastic regime of tensile deformation). Additional outcomes include the development of advanced measurement capabilities, including 3D reconstructions and subsequent registration of explicit microstructure representations using serial sectioning and HEDM.

NIST Additive Manufacturing Benchmark Series (AM Bench) [12,13]

This effort, launched in 2016, provides a continuing series of controlled benchmark measurements, in conjunction with challenge problems for the modeling community, and a conference series, with the primary goal of enabling modelers to test their simulations against rigorous, highly controlled AM benchmark test data. AM Bench curated measurement data are produced through collaborations among researchers from 10 NIST divisions and 22 outside organizations. AM Bench has provided measurement data for metals AM and polymers AM. Measurements supporting ceramics AM are underway.

Notable Outcomes: Extensive AM-focused benchmark measurement data and metadata are publicly available, covering the full PSPP range. Data releases occurred in 2018, 2022 and 2025, with further releases every three years. In 2018, AM Bench received 46 challenge problem submissions from modelers in North America, Europe, and Asia. In 2022 and 2025, AM Bench received 138 submissions and 85 submissions, respectively. In early 2026, AM Bench will hold virtual Challenge Problem Workshops for the submitting teams, once again, allowing participants to compare simulation approaches and results.

ONR Quality Made Program [251]

This effort (2018-2020) was focused on developing and demonstrating software and hardware technologies required to support the rapid qualification of critical metallic components at a reduced cost. Goals include developing, testing, and delivering validated modeling and simulation capabilities, in-situ process monitoring sensors, and control for utilizing AM from initial design to finished product including qualification of materials and processes.

Notable Outcomes: Successful hardware and software have been transitioned to Navy Warfare Centers for further development and use. This has supported a range of Naval Sea Systems Command (NAVSEA) and NAVAIR activities in the advancement of AM qualification with nickel Alloy 625, 316L, and Ti-6Al-4V. In addition, advancements were made toward anomaly detection within powder bed and directed-energy systems; this has led to maturation of in-situ sensing for process stability. Lastly, static property predictions were shown to be within ±5% of experimental values.

Transforming Additive Manufacturing through Exascale Simulation (ExaAM) [48]

As one of several topics within the Chemistry and Materials applications theme of the Exascale Computing Project (ECP) that started in 2016, ExaAM (2016-2023) was focused on accelerating the widespread adoption of AM by developing HPC codes with UQ for physics-based simulations of processing, structure, and properties, using data from AM Bench for validation. The broader Exascale Computing Project is focused on "accelerating the delivery of a capable exascale computing ecosystem that delivers 50 times the application performance of the leading 20 PF (PetaFLOPS, 10^{15} floating-point operations per second) systems and 5x the performance of the world's most powerful supercomputer." The ExaAM codes are currently running on Frontier, the world's first exa-scale computer that is located at Oak Ridge National Laboratory (ORNL).

Notable Outcomes: ExaAM resulted in the development of a number of CM tools for AM simulations, all demonstrated to scale on Frontier. Codes include melt pool-scale process modeling, microstructure simulations (grain-scale CA, and sub-grain PF approaches), and crystal plasticity property simulations. Workflow tools were developed to launch large ensembles of simulations to perform uncertainty propagation. The codes were calibrated and validated for PBF-LB processing of nickel Alloy 625 using the NIST AM Bench 2018 and 2022 datasets. Key open-source simulation and workflow tools are available at https://github.com/ExascaleAM.

NASA University Leadership Initiative (ULI) Project on Development of an Ecosystem for Qualification of Additive Manufacturing Processes and Materials in Aviation [252]

This project was active during 2019-2023, was led by Carnegie Mellon University, and was focused on the development of a qualified metallurgical process by determining a materials properties-based process window for PBF-LB AM Ti-6Al-4V using fatigue life as a metric.

Notable Outcomes: An important outcome was that fatigue defines a process window that has a sharp maximum in fatigue life which corresponds to a minimum in flaw (pore) density, i.e., the pore density and fatigue life are anti-correlated, as expected. The unanticipated result was the narrowness of the optimal range in parameter space. 4-point bend fatigue was used successfully as a high-throughput probe of fatigue behavior. Parts printed in the same model of PBF-LB machine at different institutions had similar microstructure and properties, i.e., there was little sensitivity to serial number.

NASA Space Technology Research Institute on Development of Model -based Qualification and Certification of Additive Manufacturing (IMQCAM) 2023-2028

This is a new multi-institution project led by Carnegie Mellon University and Johns Hopkins University. It has the goal of implementing a numerical DT of PBF-LB 3D printing that starts with feedstock, simulates the printing and post-processing, leading to accelerated microstructure-aware models of fatigue life. The intent is for the validated end-to-end DT to be able to predict fatigue life with fully quantified uncertainties.

Notable Outcomes: This is a new project – no major outcomes as of the time of this document's release.

DARPA Structures Uniquely Resolved to Guarantee Endurance (SURGE) 2024-2029

This new DARPA program is aimed at developing revolutionary, individual component-focused, approaches for Q&C of additively-manufactured hardware (i.e., at the point of production) under anticipated service conditions. To achieve this goal, SURGE's performers will integrate in-situ sensing technologies, physics-based process modelling and microstructure-based fatigue-life methods. A range of applications, materials and environments, beyond those relevant to aviation, will be considered.

Notable Outcomes: This is a new project – no major outcomes as of the time of this document's release.

A1.2 Examples of Government-Developed CM Software Capabilities

ExaAM: https://github.com/ExascaleAM

ExaAM was sponsored by the DOE Office of Science and National Nuclear Security Administration and was aimed at developing an Integrated Platform for Additive Manufacturing Simulations (IPAMS), specifically focused on supporting PBF-LB AM. The platform integrates high-fidelity mesoscale simulations into continuum process simulations to accurately predict microstructure and properties based on process and location-specific conditions. The approach involves using various simulation techniques at different scales, culminating in a workflow that simulates complex microstructures that are often associated with the powder-bed processes. Typically, thermomechanical FEA models are used at the macroscopic part scale; finite volume or FEA models are used at millimeter scales for fluid dynamics and heat transfer to capture the melt pool dynamics and solidification; mesoscale approaches (e.g., discrete elements, CA, KMC, or PF models) are used at the micron scale to simulate melting, solidification, and microstructure formation; and polycrystal plasticity models are used to develop the microscale mechanical property relationships. Specifically, the workflow includes AdditiveFOAM, a powder layer melt-refreeze model, ExaCA, a microstructure evolution model, and ExaConstit, a crystal plasticity FEA model to link process-specific microstructure to properties.

LAMMPS: https://www.lammps.org
LAMMPS (an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator) is a classical molecular dynamics code with a focus on materials modeling developed by the DOE. LAMMPS uses interatomic potentials for solid-state materials (metals, semiconductors), soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale. LAMMPS can be executed on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain, can exploit accelerated performance on CPUs, GPUs, or Intel Xeon Phi processors, and is designed to be easy to modify or extend with new functionality. LAMMPS is distributed as an open-source code.

SPPARKS: https://spparks.github.io
SPPARKS (an acronym for Stochastic Parallel PARticle Kinetic Simulator) is an open-source simulation package from the DOE's Sandia National Laboratories that includes a range of parallel Monte Carlo implementations for on-lattice and off-lattice models. Numerous sub-applications are included with SPPARKS. The code has been used to accurately simulate grain growth and microstructure evolution during welding, AM, and heat treatment.

MOOSE: https://mooseframework.inl.gov
Moose (an acronym for Multiphysics Object Oriented Simulation Environment) is an open-source, parallel FEA framework developed by the DOE's Idaho National Laboratory for solving coupled multi-physics simulations. MOOSE offers a wide range of physics modules spanning the fields of solid mechanics, heat conduction, thermodynamics, chemistry, fluid dynamics, electromagnetics, nuclear physics, and more. The framework includes an ecosystem of tools that accelerate the new development and coupling of physics governing equations, such as highly parallelizable solution methods, automatic differentiation for simplified model development, and visualization. An active open-source community continues to deploy major developments to the software and apply the framework to many manufacturing processes, physical processes, and structural applications.

DREAM3D: https://dream3d.bluequartz.net
DREAM3D (an acronym for Digital Representation Environment for Analysis of Materials in 3D) is a comprehensive open-source software suite developed by Blue Quartz Software LLC and AFRL to create customized workflows for processing and analyzing diverse data sources used throughout the field of materials science and engineering. Core features of the software include 3D reconstruction and registration of microstructures from experimental data, synthetic microstructure generation, computation of microstructural statistics, image processing algorithms, interoperability with industry-standard data formats, and data visualization. DREAM3D provides a user-friendly interface and an extensible data structure in a non-proprietary format, which also maintains a complete record of all applied data processing steps enabling the transferability and reproducibility of materials data across the community.

PRISMS: http://prisms-center.org/#/home
PRISMS (an acronym for Prediction of Realistic Integrated Structure Materials Science) is a DOE-funded open-source software framework designed to accelerate the development of new

materials by simulating their properties at multiple length scales, from atomistic to macroscopic length scales. This capability is achieved by integrating a suite of tools including but not limited to: 1) DFT, 2) statistical mechanics, 3) PF, 4) CP, and 5) continuum mechanics solvers. Furthermore, the suite of tools within PRISMS provides scalable HPC capabilities for solving large-scale multi-physics problems and model integration across different length scales.

Appendix II A Worked Example of UQ

The following example was taken from a recent paper [253] in which the authors explore UQ for a particular aspect of metals AM that affects many of the outcomes of interest to CM4QC, namely, the 3D melt pool geometry. The authors constructed a surrogate model for the 3D melt pool, relying on experimental data from AM Bench. They used Bayesian methods to re-calibrate the surrogate model, i.e., to improve its accuracy. As noted previously, the 3D melt pool affects many aspects of metals AM. For example, the variance in melt pool shape contributes to porosity wherever adjacent melt tracks fail to overlap and fully melt the powder, leading to LOF pores. Because of the highly non-spherical nature of such pores, they have a particularly deleterious effect on fatigue performance via their strong stress concentration effect. As seen below in Figure A2.1, the approach fits a surrogate model to the available experimental data for melt pool characteristics. This method is, of course, subject to substantial uncertainty, which they reduce via a sequential calibration and validation (SeCAV) approach. They simplify the sources of experimental variation to five variables, *viz.*, pre-heat temperature, laser absorptivity, spot radius, convection coefficient (heat transfer), and ambient temperature. They extract melt pool variability from the AM Bench data to update the distributions of the various sources of uncertainty, determining in the process that variables such as spot size and absorptivity each contribute substantial uncertainty. These distributions are shown for both the prior versions and the re-calibrated results in Figure A2.2, which illustrate the importance of all five variables and the extent of the re-calibration. Finally, the authors present an experimental validation of the re-calibrated model against the AM Bench data in Figure A2.3. It is important to note that they actually used three different methods which they term as “Direct1,” “Direct2,” and “SeCAV” of which the latter provided the best agreement for all seven datasets. What is particularly useful in this example is that the article addresses the porosity that is expected to result from melt pool variability, which is mentioned previously as an opportunity for full-field simulations of laser melting but where the expense of such simulations clearly motivates a need for reduced-order models.

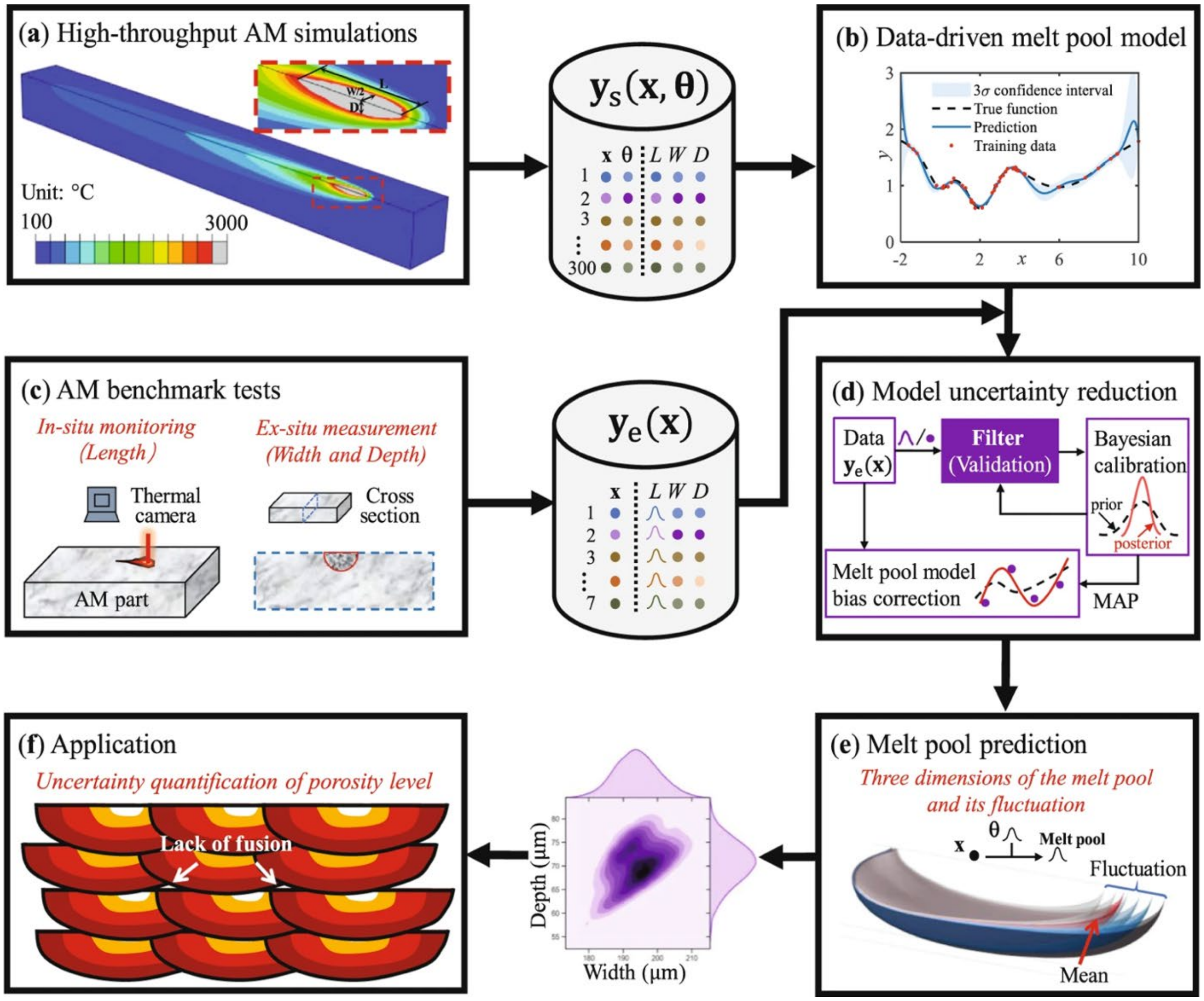


Figure A2.1 AM thermal simulations at 300 sampling points are performed to provide a large training dataset of the pool length, width, and depth; **b** a data-driven melt pool surrogate model is built based on the simulation-obtained data; **c** experimental data from AM Bench measurements are used for uncertainty reduction of the melt pool model. The measured fluctuation information of the melt pool, represented by the interval data of pool length, are used in the calibration. These experimental data in three dimensions of the melt pool are obtainable through a close collaboration between in-situ monitoring and ex-situ measurement; **d** a sequential Bayesian calibration method (i.e., SeCAV) is adopted to systematically quantify the uncertainty sources by filtering the misleading information contained in experimental data. The model bias of the as-built melt pool surrogate model is also corrected; **e** upon validation, the calibrated melt pool surrogate model is capable of efficiently predicting all three dimensions of the developed melt pool, as well as its fluctuation caused by uncertainty sources; **f** to illustrate the practical usefulness of the developed melt pool surrogate model, the predicted pool width and depth information can be incorporated into a porosity predictive model, to investigate the uncertainty of porosity formation and thus the variability in porosity level among AM parts. After Wang et al. [253]; cross-refs omitted.

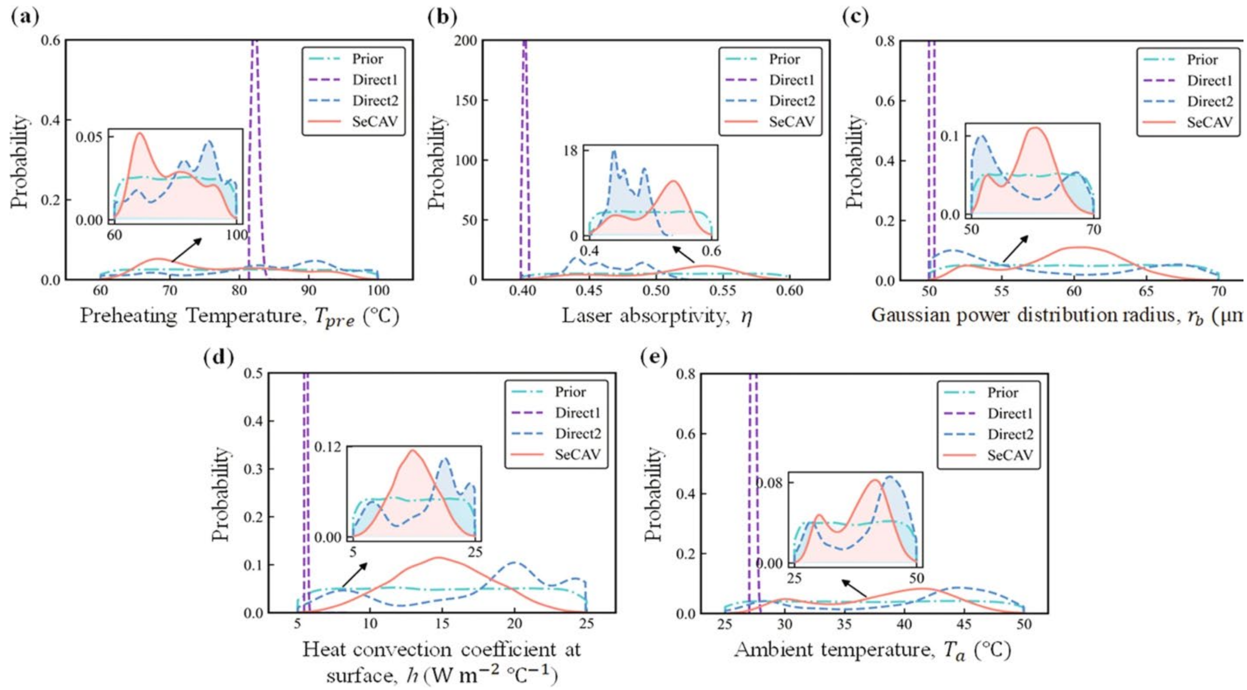


Figure A2.2 The uncertainty source parameters, including **a** preheating temperature, **b** laser absorptivity, **c** Gaussian power distribution radius, **d** heat convection coefficient, and **e** ambient temperature, see a significant uncertainty reduction, presenting as a more concentrated distribution after experimental calibration. After Wang et al. [253]; cross-refs omitted.

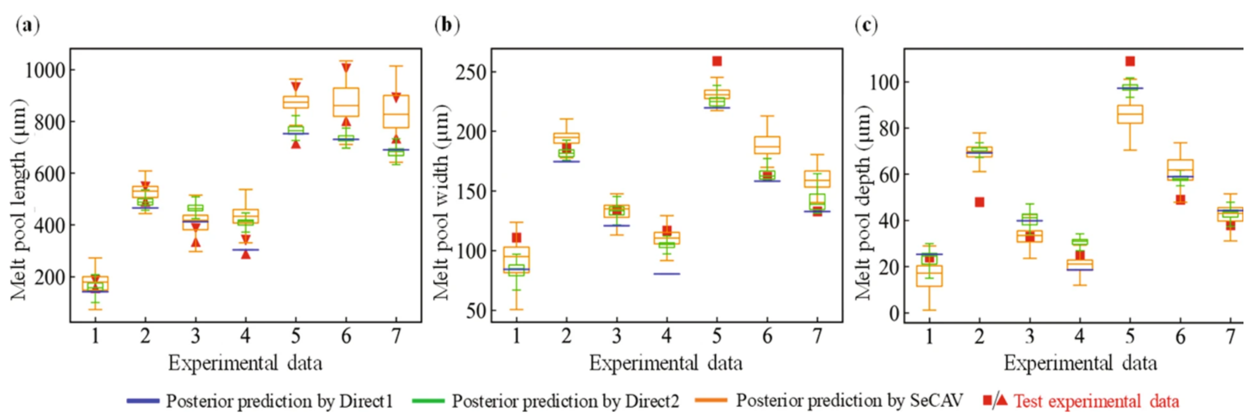


Figure A2.3 The three calibrated models are compared for predicting: **a** pool length, **b** pool width, and **c** pool depth. It should be pointed out that box-plots in blue should not be mistaken as lines; instead, they just reflect near-zero fluctuations of pool geometry predicted by the calibrated surrogate model using the Direct1 method. After Wang et al. [253]; cross-refs omitted.

Appendix III Simulation Maturity Level Spreadsheet Cell Descriptions

A3.1 Application and Model Definition (Column C)

SML 1, Application and Model Definition

Application intent defined. Models defined. Model inputs and outputs defined.

Tasks at SML 1 are all definition focused. Since any assessment of SML is application dependent, the intended application must be defined. Next, the primary models used for the simulation need to be described, along with detailed descriptions of the expected model inputs and outputs.

SML 2, Application and Model Definition

Significant sub-models defined. All sub-model inputs and outputs defined.

Tasks at SML 2 are focused on providing more granular details on the intended models, including descriptions of any sub-models that are used for the simulations. Descriptions of the expected sub-model inputs and outputs are also needed. Clearly, lower-level sub-models that interface with higher level sub-models should have corresponding inputs and outputs.

SML 3, Application and Model Definition

Recommended applications and limitations defined.

For SML 3, further details are needed on the recommended applications. This includes expected boundary conditions for the models and sub-models, required parameter inputs, and assessments of the necessary accuracy and precision the models need to achieve to satisfy the intended application(s).

SML 4, Application and Model Definition

Recommended applications and limitations updated.

Applications are expected to rely more heavily on simulations as SML increases. Thus, for each higher SML level, a thorough fine tuning and reassessment of the applications, models, sub-models, and simulation limitations is needed.

SML 5, Application and Model Definition

*Recommended applications and limitations updated (*suitable for all intended use cases*).*

Applications are expected to rely more heavily on simulations as SML increases. Thus, for each higher SML level, a thorough fine tuning and reassessment of the applications, models, sub-models, and simulation limitations is needed.

A3.2 Range of Applicability (Column D)

SML 1, Range of Applicability

Range of applicability of the physics and data-based models are defined to satisfy the intended application.

Identify all required physics, data requirements, and numerical methods.

SML 2, Range of Applicability

All input parameter ranges and the effects of their interactions specified to satisfy the intended range of applicability.

SML 2 Verification (column F) and Validation (column H) must be completed and used to determine parameter ranges and interactions.

SML 3, Range of Applicability

Limitations implemented to control use or warn user if inputs & outputs are outside of range. Sub-model outputs generated and assessed over required ranges.

Limitations implemented in simulation software or through user procedures. SML 3 Verification (column F) and Validation (column H) completed and used to test parameter ranges, interactions, and outputs for sub-models.

SML 4, Range of Applicability

Models, sub-models, and their interfaces assessed for all intended input ranges and use cases.

SML 4 Verification (column F) and Validation (column H) completed and used to test parameter ranges, interactions, and outputs for models, sub-models and their interactions.

SML 5, Range of Applicability

Full range of applicability updated for all intended use cases.

Continued refinement of the user guide consistent with additional benchmark cases and publication of supporting data. Additional activities performed at SML 5 are documented as detailed in the Documentation Activity Tracker.

A3.3 Supporting Data (Column E)

SML 1, Supporting Data

Supporting data requirements identified and documented in coordination with Verification, Range, UQ, Validation, and Risk tasks.

The nature of necessary Supporting Data has been considered and an initial estimate of requisite data, both in terms of nature and quantity, has been formulated. These data serve several purposes, so this step must be executed in concert with planning activities outlined in parallel tasks. Not all desired or required data may be available at this stage, but this critical planning step should identify such situations to inform parallel tasks.

SML 2, Supporting Data

Some supporting data available. Data documentation and archival plan developed. Access control and authentication plan in place for cases where broad accessibility is not feasible. FAIR Principles considered.

Some supporting data have been identified, but data generation via measurement activities may be ongoing. Documentation includes a description of the techniques used to generate and reduce the data, as well as confidence bounds/uncertainty of measured data, the overall range covered by the dataset, the quantity of data, and description of train-test and/or calibrate/validate splitting as applicable. There is continuous coordination with other tasks, in particular those in the Validation and Uncertainty Quantification categories.

SML 3, Supporting Data

Supporting data adequate to perform SML 3 Verification, Validation, and UQ tasks over a limited range of application. All supporting data identified, documented, and archived.

The available Supporting Data are sufficient to allow necessary quantitative comparisons for sub-model outputs on specific, limited test cases. This includes performing UQ analyses and quantification of sensitivities. Data generation may be ongoing for a broader range of use cases.

SML 4, Supporting Data

Supporting data adequate to perform SML 4 Validation and UQ tasks for several relevant use cases. All supporting data identified, documented, and archived.

Data generation activities are completed in order to expand the Supporting Data beyond the limited cases from SML 3 to cover several relevant use-cases. Furthermore, data are sufficient to assess performance of the full model, not just sub-models. Expansion of documentation and data archive covers these additional cases.

SML 5, Supporting Data

Supporting data documentation and archive maintenance performed as additional experience from SML 5 Validation or UQ tasks becomes available.

Maintenance of existing Supporting Data archives ensures persistent access for authorized parties. The archive may be expanded to include additional use cases, but all previous Supporting Data remain in place.

A3.4 Model Verification (Column F)

SML 1, Model Verification

Code and solution verification plan developed. Preliminary and informal code verification performed. Version control strategy selected. QOIs for solution verification identified.

A working simulation software code has been demonstrated to give physically reasonable results. Non-rigorous testing (e.g., qualitative assessment of results or comparison with previous codes) has been performed. Theoretical convergence orders for numerical methods used are known. Code verification problems with exact solutions have been identified or created using the method of manufactured solutions [183]. QOIs to evaluate solution verification have been defined.

SML 2, Model Verification

Rigorous code verification completed for individual sub-models by demonstrating theoretical order of accuracy and/or convergence rates, where applicable. Unit testing implemented for sub-models. Version control implemented, documented, and archived.

Spatial and temporal convergence calculated for individual sub-models, with convergence rates demonstrated to match expected theoretical order of accuracy in mesh and time step size for discretized formulations. Unit tests (small calculations with known output or solutions) have been implemented for sub-models or functions. Simulation software changes are tracked through a version control system with a clear strategy for labeling versions and branches.

SML 3, Model Verification

Rigorous code verification completed for relevant combinations of sub-models by demonstrating theoretical order of accuracy and/or convergence rates, where applicable. Refinement studies completed for problems of interest, with mesh convergence demonstrated. Regression testing implemented.

Code verification including spatial and temporal convergence tests are complete for all relevant combinations of sub-models, and the expected convergence rate has been demonstrated within the asymptotic limit of small grid or time step size for discretized formulations. For the application problem of interest, mesh or time step refinement studies are performed to qualitatively demonstrate convergence of QOIs with refinement. Regression tests, including both unit tests and code verification tests, are run frequently to ensure code changes do not cause unexpected changes in results; tests are implemented on one or more platforms (where a *platform* refers to a specific combination of compiler, operating system, and hardware). Developers run regression tests before code changes are committed or archived. Code coverage of regression tests may be incomplete.

SML 4, Model Verification

Numerical error, including discretization error where applicable, quantified for QOIs in problem of interest and deemed small compared with validation measurement error. Regular regression testing for one or more platforms.

Solution verification has been performed using a technique such as Richardson extrapolation [183] to estimate the convergence rate and quantify the discretization error for QOIs. Discretization error is shown to be negligible compared with measurement error in validation testing. A suite of regression tests is run frequently, with a goal of complete code coverage.

SML 5, Model Verification

All numerical error sources (including round-off, discretization, and iteration tolerance) are understood and quantified for QOIs. Automated and documented regression testing system implemented for all relevant platforms.

For the problem of interest, all numerical error sources, including roundoff (floating-point) error, discretization error in time and space, matrix solve tolerance, and iteration error, have been quantified, and total numerical error is small compared with validation measurement error. Regression tests are performed upon code changes, and regularly at a given frequency (e.g., nightly). Tests are regularly performed for all relevant platforms and operating systems. Sub-model coverage for each regression test in the suite is understood and documented.

A3.5 Uncertainty Quantification (Column G)

SML 1, Uncertainty Quantification

Parameters of interest and UQ plan defined.

Input parameters and QOIs have been identified and a UQ plan has been developed and approved by relevant stakeholders. Sources of data and data collection efforts identified. QOIs are defined as direct model outputs (e.g., temperature profile) as well as derived quantities (e.g., melt pool volume).

SML 2, Uncertainty Quantification

Deterministic sensitivity study performed on selected input parameters to quantify influence on QOIs. One-at-a-time, DoE, and expert opinion coupled with sensitivity analysis performed for input parameters. Parameters and range of outputs identified.

A progression of exploratory efforts from an individual (one-at-a-time) input parameter study to a robust DoE, followed by selective variations guided by expert opinion have been performed. A DoE is a systematic means of efficiently quantifying the variation in QOIs as a function of variations in input parameters. Data, expert opinion, and prior experience are used to quantify variations in input parameters. Sensitivities of the QOIs to the input parameters are quantified. Sensitivity analysis defines critical parameters and the anticipated range of QOIs.

SML 3, Uncertainty Quantification

Random variables identified and quantified. Probability-based UQ analysis performed for sub-model outputs. Probabilistic sensitivities quantified.

Uncertainty Quantification performed on sub-models. Sub-models are numerical routines which typically capture a single aspect of the needed physics (e.g., laser fusion and material state, thermal history, microstructural evolution in response to thermal history, crystal plasticity modeling, etc.). Statistical (aleatoric) variations in relevant input parameters have been estimated with quantified confidence. These variations have been used to calculate the expected variation and probabilistic sensitivities for sub-model QOIs. Probabilistic sensitivities account for both the deterministic sensitivity and statistical variation of input parameters on the sub-model QOIs. These variations in sub-model QOIs may be used to infer the variation and probabilistic sensitivities for the full model QOIs. Epistemic (model form) uncertainty associated with sub-model may be assessed by quantifying the variation in sub-model QOIs with changing physics and model assumptions/approximations.

SML 4, Uncertainty Quantification

UQ analysis per SML 3 performed and documented for the QOIs from full model for all relevant use cases. Probability results available for validation for all QOIs.

Probabilistic-based UQ of the full model QOIs is performed by propagating uncertainties from the sub-models in SLM 3 through the full model. Uncertainty analysis is performed over the range of intended use cases of the full model. The QOI uncertainty may be separated into its aleatoric and epistemic components.

SML 5, Uncertainty Quantification

FAIR modeling & measurement data summarized. Results compared against industry-accepted, benchmark or standard cases as available. Results documented and reviewed for validation for all QOIs.

FAIR principles are used to document the model UQ. Documentation must present the UQ approach, method, and results, including industry-recognized use cases and standard benchmarks where appropriate. Reporting should be peer reviewed and available to all stakeholders. Supporting data should be readily discoverable and accessible, along with accompanying documentation that facilitates traceability, reproducibility, and applicability.

A3.6 Model Validation (Column H)

SML 1, Model Validation

Validation requirements defined for selected application.

The validation requirements are defined based upon the application, the range of applicability, and the performance risk assessment. At this SML level, detailed measurement plans are not required, but preliminary identification of needed measurement data and selection of measurement methods should be carried out.

SML 2, Model Validation

Validation plan developed for both intended use and all sub-models.

Validation plans must include 1) identification of the validation data needs, 2) identification of the data sources, 3) measurement plans for acquiring needed data not available through public sources, and 4) plans for conducting the required validations using the measurement data, measurement uncertainties, model predictions, model UQ, and quantitative validation metrics.

SML 3, Model Validation

Sub-models validated against established benchmarks or equivalent data. Model output similarly validated for specific cases.

Characteristics of successful benchmark measurements include 1) highly controlled measurements that target specific modeling needs, 2) comprehensive characterization of boundary conditions to minimize use of fitting parameters by the modeling teams, 3) determination of required input parameters or inclusion of model calibration data, 4) measurement UQ to the greatest extent possible [139–145], 5) quantitative metrics for comparing the measured and simulated results, and 6) FAIR data management [14,15]. Established benchmark datasets for metal AM include those from AM Bench led by NIST [12,13]. In general, the high cost for acquiring and curating benchmark measurement data severely limits the number of public benchmark measurements that can be conducted so the demand for such high-quality validation data is always greater than the supply. Equivalent data must be acquired following practices similar to those described above for benchmark data. Additional useful discussion about benchmark measurements for model validation may be found in Section 6.

SML 4, Model Validation

Model and sub-models validated for all relevant use cases using established hierarchical benchmarks or equivalent data.

To validate a computational model that includes sub-models, two feasible approaches can be effective: hierarchical benchmarks and validated sub-models with extensive additional validation of model predictions.

Hierarchical benchmarks are a new concept for metal AM model validation where a series of coupled benchmark measurements span a single complete AM process, from feedstock characterization, through the build and post-build processing, mechanical behavior, and interaction with the operating environment. This allows the hierarchical coupling of the sub-models to be validated. The key advantage of this approach is the seamless connection between the validation of the different sub-models and the validation of the model.

Hierarchical benchmarks are exceedingly large and costly, with extensive collaborations needed between different measurement organizations. It is therefore impractical to require the use of such benchmarks for validating application models. An alternative is to supplement the sub-model validation described for TRL 3 with validation of model outputs over a sufficiently wide range of conditions to ensure that the hierarchical structure of the full model behaves as expected.

SML 5, Model Validation

Model fully validated over range of applicability using validation data, operational performance data, and experience.

The validation data should be reassessed to ensure that the required scope of the simulations for the intended application is adequately validated. This may include incorporation of operational performance data and experience with the operational system.

A3.7 Performance Risk Assessment (Column I)

SML 1, Performance Risk Assessment

Identify risks associated with CM use for application. Complete an initial Risk Assessment.

Document potential sources/categories of risk and consequences associated with use of the model/sub-model. Document potential mitigation tasks for all high-risk items.

SML 2, Performance Risk Assessment

Risk assessment plan should be fully developed taking validation and UQ plans into account. Mitigation plans should also be fully developed.

Finalize sources/categories of risk and consequences associated with use of the model/sub-model. Note that the risk-consequence matrix should inform and guide V&V requirements. High-risk sources will have to be managed to reduce risk to acceptable levels.

SML 3, Performance Risk Assessment

Preliminary risk assessment conducted with input from validation and UQ analysis. Mitigation activities should be reviewed and assessed to reduce likelihood of occurrence and/or consequences to level acceptable for the application.

Document level of risk assessments associated with all categories, complete and accurate to a high degree of probability. Manage High-Risk / High-Consequence items to reduce risk or implement alternate methods.

SML 4, Performance Risk Assessment

Risk for CM use assessed for application in component and process development and testing stages.

Document the results of multi-disciplinary risk assessment, including responsible stakeholders or customers, and non-advocate experts. Address any major concerns or actions which arise from this activity. High-Risk / High-Consequence items should be mitigated to lower levels.

SML 5, Performance Risk Assessment

Risk assessed for application Q&C activities.

High-Risk / High-Consequence items should be at low acceptable levels and should be monitored to maintain low risk.

A3.8 Documentation (Column J)

SML 1, Documentation

Outcomes of SML level 1 planning and description activities for other SML criteria documented.

Tasks at SML 1 focus on documenting the model definition, as well as criteria and planning activities for columns Supporting Data, Model Verification, Range of Applicability, Uncertainty Quantification, Model Validation, and Performance Risk Assessment. The formats for these are not specified, but each respective SML attribute section describes key details that shall be included in this documentation.

SML 2, Documentation

User guide initiated, SML 1 plans updated, and SML 2 activities documented.

Documentation at SML 2 includes a draft version of a user guided for refinement in later SMLs. Plans developed and documented at SML 1 shall be updated to reflect changes consistent with SML 2 for activities in other categories (i.e., description of supporting data identified, creation of validation plan, UQ sensitivity analysis results, etc.)

SML 3, Documentation

User guide developed and documented. Licensing and support strategy considered, if applicable. SML 3 activities documented.

A more functional user guide describing tool use, current range of applicability, verification cases, as well as limited validation cases shall be written. Licensing and support strategies, if applicable, shall be available for review by potential users. Continued updates to documentation from prior levels are expected, as well as documentation of additional activities performed at SML 3, as detailed in the Documentation Activity Tracker.

SML 4, Documentation

User guide updated to reference supporting data, UQ analysis, V&V cases. Licensing and support implemented, if applicable. SML 4 activities documented.

The user guide shall be refined to include the increasing breadth of range of applicability and validation cases, as well as progress in UQ. Additional activities performed at SML 4 are documented as detailed in the Documentation Activity Tracker.

SML 5, Documentation

User guide updated. SML 5 activities documented.

Continued refinement of the user guide consistent with the addition of additional benchmark cases and publication of supporting data. Additional activities performed at SML 5 are documented as detailed in the Documentation Activity Tracker.

Appendix IV Abbreviated Documentation Activity Tracker

For the fully detailed documentation activity tracker, see the worksheet "Documentation Activity Tracker" in Simulation_Maturity_Level_Spreadsheet_With_Appendices.xlsx

SML	Item
1	Application and model definitions documented
	Intended range of applicability documented
	Supporting data requirements documented
	Code verification plan documented
	Solution verification plan documented
	Version control strategy identified and documented
	Verification Quantities of interest defined, documented
	Parameters of interest listed
	UQ plan documented
	Validation requirements documented
	Initial risk assessment documented
1	This tracker updated
2	Sub-models defined and documented
	Sub-model inputs/outputs documented
	Input parameter ranges and effects documented
	Any extant supporting data documented
	Supporting data access control plan documented
	FAIR principles considered
	Code verification cases documented
	Sub-model unit tests documented
	Any changes to version control strategy documented
	Sensitivity analysis results documented, including range of outputs
	Validation plan documented
	Risk Assessment and Mitigation plans documented
	Draft user guide written
2	This tracker updated
3	Applications and limitations documentation updated
	Range limitations documented
	Sub-model output assessment documented
	Supporting data description and archive manifest updated
	Code verification case documentation updated
	Regression testing cases documented
	Random variables documented
	Probability based UQ analysis outcomes documented for sub-models

	Sub-model validation performance documented
	Model validation performance documented for specific cases
	Preliminary risk assessment documented
	Updates to mitigation activities documented
	User guide updated
	Licensing strategy documented
	Support strategy documented
3	This tracker updated
	Applications and limitations documentation updated
	Model and sub-model range limitations documents updated
	Adequacy of supporting data for Validation and UQ documented
	Supporting data archive manifest updated
	Discretization errors documented
	Regression testing cases documented, updated
4	UQ analysis outcomes documented for full model, all test cases
	UQ validation documented
	Model and sub-model validation performance documented across relevant cases
	Risk assessment documented for development and testing stage
	User guide updated
	Licensing, support documents available
4	This tracker updated
	Applications and limitations documentation updated
	Range of applicability updated across relevant use cases
	Supporting data documentation updated/maintained
	All numerical error sources documented
	Regression testing documentation updated
5	UQ applied benchmark cases documented
	Model performance compared to requirements for intended use
	Benchmark validation case outcomes documented
	Risk quantification documentation updated to include application Q&C activities
	User guide updated
	Verification and validation cases fully documented
5	This tracker updated

Appendix V Example Success Stories: Computation of Residual Stress

A5.1 Introduction

It is useful to look at historical precedents in related fields to see if valuable lessons may be learned that could provide guidance to the current focus. One such example is the development and introduction of residual stress simulation using FEA.

Between the mid 1950's and the mid 1970's, FEA grew from its origins in structural analysis into one of the most active areas of research in numerical analysis/computational methods [254]. Much of this early growth was driven by aviation applications. For example, early work by Turner et al. in 1959 was driven by a need to analyze delta wings [255]. By the mid 1980's, residual stress analysis using FEA was widespread, but results were inconsistent and not trusted for mid- or high-TRL applications. This landscape changed in 1988 when the first public benchmark measurements for residual strains were introduced for plastic deformation of metals. The results were game changing. As described by Wagoner and Hora [256], "No program in existence at that time, commercial or research, achieved a physically reasonable result for the simplest forming operations that were simulated." This result launched major improvements in material models and simulation programs. Within five years, most of the automotive companies were using these improved codes to dramatically decrease the trial-and-error burden of designing stamping dies, with related costs decreasing by 80% for some manufacturers [256]. Perhaps even more importantly, the critical importance of validating modeling results for commercial applications was firmly established.

A5.2 Example of the Effective Use of Predictive Tools in the Aviation Industry

Residual stresses are ubiquitous in manufactured metal components, and they can seriously impact the manufacturability and performance of the part. Residual stresses can develop whenever plastic deformation occurs and such stresses are commonly produced during welding, metal forming, forging, casting, AM, and nearly every other manufacturing approach. The ability to accurately simulate the formation of residual stresses during manufacturing allows process designers to alter the magnitude and distribution of residual stresses in the parts, and to directly compensate for any resulting part distortion.

This sub-section describes a successful USAF program focused on establishing methods for linking predictive tools with component design functions, with a primary application to nickel-base superalloy engine disk components [257,258]. Residual stresses in these components, emerging from various manufacturing stages, can pose significant challenges in maintaining structural integrity and performance. The USAF funded a FEP aimed at addressing this issue [257,258]. This FEP focused on establishing methods to link predictive tools with component design functions, with an emphasis on incorporating residual stress considerations into the manufacturing, design, and structural analysis of aeroengine disks. Critical elements included extensive validation testing and UQ analysis for both the measurement and simulation results. This program demonstrated the effectiveness of including CM approaches in the engineering design loop by enabling a weight reduction of over 30%.

For this FEP, a team of aerospace OEMs and suppliers that consisted of Rocketdyne, General Electric, Honeywell, Rolls Royce, Pratt & Whitney, Boeing, and Allegheny Technologies executed a collaborative effort working towards standardizing protocols for residual stress management in nickel-base superalloy components. By developing an ICME infrastructure, the program optimized manufacturing parameters while meeting rigorous disk design criteria. This multi-disciplinary approach connected materials and process models with structural analysis tools, enabling informed decision-making throughout the supply chain [257,258].

The FEP addressed inherent challenges associated with uncertainty in modeling results and residual stress measurements through a UQ task. Focused measurement plans were developed to update and validate modeling tools, ensuring accuracy and reliability in predicting residual stress states. Multiple measurement methods were conducted including hole drilling, contour, X-ray diffraction, and neutron diffraction to provide the accuracy and precision needed. Advanced computational tools such as Design Environment for Forming (DEFORM) and ANSYS were leveraged to simulate residual stress states and disk growth, facilitating sensitivity analyses and optimization of manufacturing processes.

The program demonstrated the effectiveness of ICME workflows and highlighted integrated modeling tools that streamlined component design and manufacturing process simulations. Isight software served as a central platform for linking a variety of modeling tools and automating simulation tasks, enhancing collaboration between OEMs and suppliers while ensuring the integrity of intellectual property.

Furthermore, the program emphasized the importance of optimizing disk designs while considering probabilistic design constraints such as residual growth. Monte Carlo simulations were employed to introduce variation into growth predictions, enabling the determination of optimal designs that balance weight, performance, and residual stress considerations. A weight reduction of over 30% was achieved in the optimized nickel Alloy 718 disk over the nominal baseline design.

Hence, the FEP program represents a significant step forward in incorporating residual stress considerations into the design and manufacturing of nickel-base superalloy engine disk components. Through the development of ICME infrastructure, UQ methodologies, and optimization workflows, the program demonstrated a holistic approach towards enhancing the design and manufacture of aerospace components. This ICME framework could be further extended to assessing location-based properties, such as microstructure, tensile strength, and creep, to improve component designs.

A5.3 Advances in residual stress and strain predictions for nickel-base superalloy parts produced using PBF-LB

As described in Sections 5.2.1 and 8.3, most metal AM processes produce parts with residual stresses that are large enough to adversely affect both the build process and the component mechanical behavior. As demonstrated in Section A5.2, the ability to accurately model such stresses is a key capability that can contribute to efforts to alleviate such deficiencies. Although residual stress modeling has a long history and is used routinely for a wide range of manufacturing approaches, its use for AM is relatively recent and is lower on the TRL scale.

Recent residual stress modeling predictions submitted to public benchmark challenge problems have demonstrated that these simulation capabilities are maturing to the point where they could be incorporated into higher TRL endeavors. In 2018, AM Bench conducted highly controlled PBF-LB builds of nickel-base superalloy nickel Alloy 625 test objects and performed extensive in-situ and ex-situ measurements with all data made available to the public [12]. These measurements included residual elastic stresses and strains measured using synchrotron X-ray diffraction, neutron diffraction, and mechanical release, along with part deflection measurements after the parts were partially cut from the build plate. Figure A5.1 shows elastic strain components measured from 2248 sample locations using synchrotron X-ray diffraction [259].

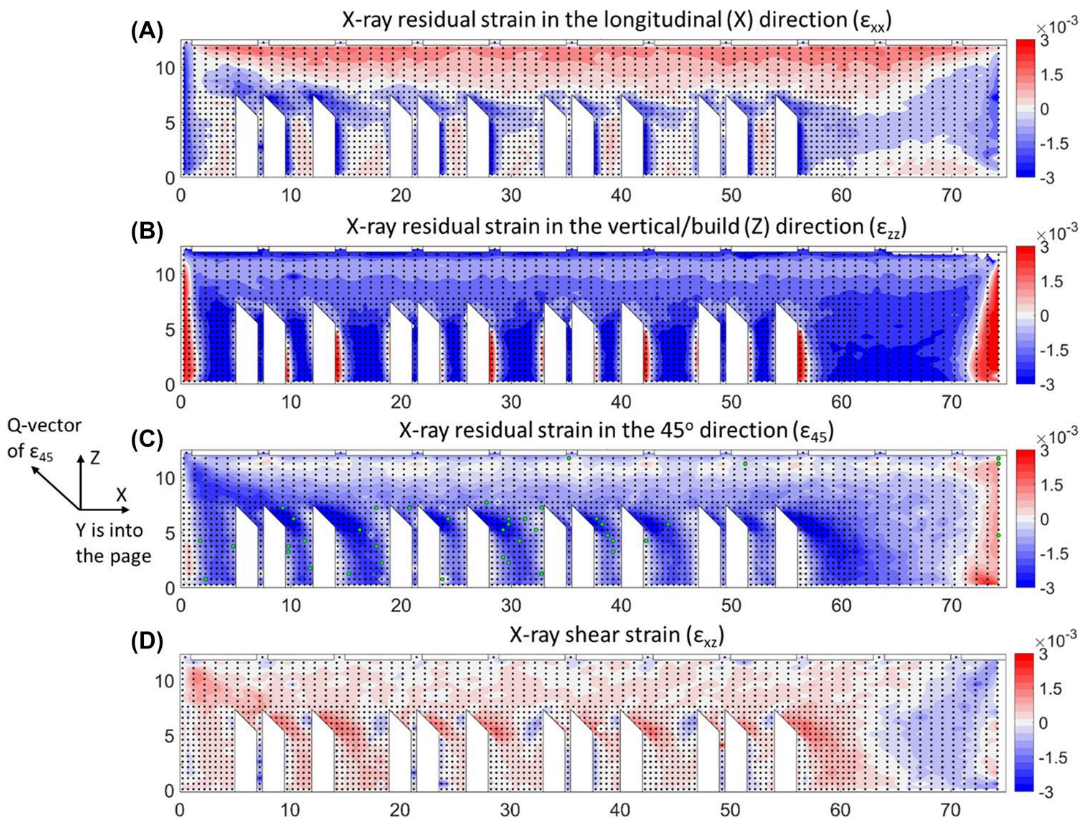


Figure A5.1: Residual elastic strains in AM-built nickel Alloy 625 parts measured using synchrotron X-ray diffraction for AM Bench 2018. Taken from Ref. [259].

Three months prior to the data release, AM Bench posed a series of challenge problems to the AM modeling community, including challenges to predict the residual elastic strains and the part deflections. As described in the AM Bench 2018 Outcomes publication [12], the best submitted simulation results were in qualitative agreement with the measured elastic strains, but the accuracy of the predictions varied considerably throughout the part, with some regions deviating by approximately 100%. The part deflection predictions also deviated from the experimental results, with none of the submitted simulation results coming close to the measured values as shown in Figure A5.2.

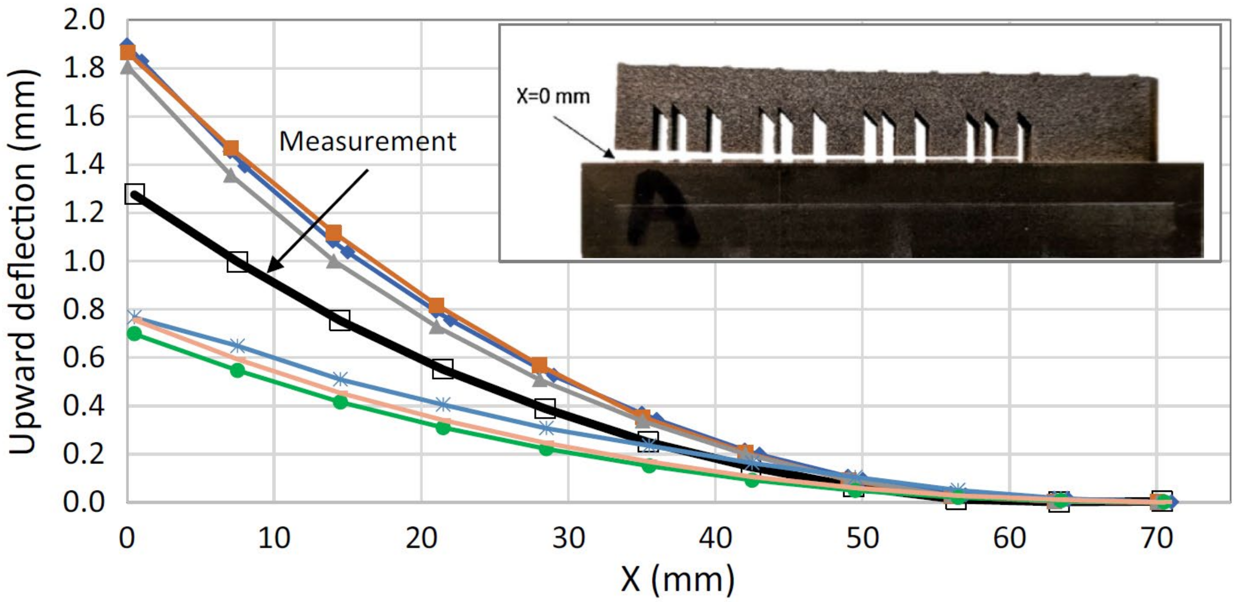


Figure A5.2: Measured and simulated part deflections for the AM Bench 2018 part deflection challenge problem. The inset photograph shows the measured nickel Alloy 625 AM-built part. Taken from Ref. [259].

In 2022, AM Bench released a similar set of challenge problems for AM builds of nickel Alloy 718 using very different build parameters and laser scan path from 2018 [13]. Figure A5.3 shows the measured residual elastic ZZ strains compared with the best submitted simulation result [12]. The submitted residual strains were considerably improved over those received four years previously. As described in Ref. [88], "the best AM Bench 2022 strain predictions were nearly indistinguishable from the measured results." Deviations were generally below 10% strain. In contrast, the submitted deflection predictions showed more modest improvement from 2018. Since AM Bench provided no calibration data for either the residual strains or mechanical deflection, it is likely that real-world simulations that include such calibration data would produce results suitable for at least some Q&C applications. Of course, the AM Bench comparisons shown here reflect only simulations for nickel-base superalloys produced using PBF-LB with a single part geometry. Considerable work is needed to validate such simulations for real-world use. Section 6 provides suggested guidance for such validation.

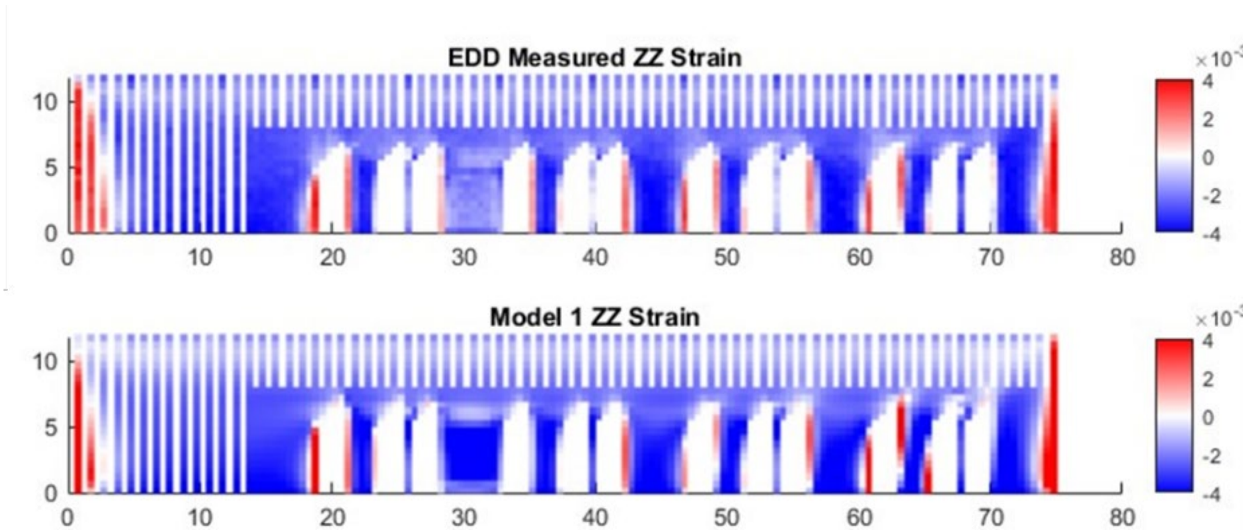


Figure A5.3: (Top) Residual elastic strains in AM-built nickel Alloy 718 parts measured using energy dispersive synchrotron X-ray diffraction (EDD) for AM Bench 2022. (Bottom) Submitted elastic strain simulations corresponding to the measurements shown at (Top). Taken from Ref. [88].

Hence, it is likely that residual stress predictions are mature enough for predicting bulk stresses in parts and should be in regular use. These predictions are very suitable for distortion and overall part average stress states as is needed for AM parts. However, the fidelity of residual stress predictions, and associated UQ, are likely not accurate enough today to be used directly in life predictions, especially damage tolerance predictions where accurate residual stress gradients must be determined locally in a part for superposition with service stresses.

Appendix VI Supporting Comments for Table 9.1

Thematic Area	Topic	Current Status	Development Difficulty	Required Input and Validation Data, and Associated Challenges	Examples of Investment Opportunities
Physics – Process	1. LOF porosity [89]	Peer-reviewed literature contains evidence that the geometric model is valid but melt pool variability is not well characterized and should also be considered.	Straightforward for simple geometric approaches. More complex as sources of variability are included.	Porosity size distribution and three-dimensional locations with respect to process conditions and feedstock characteristics, particularly as capturing variability.	Although the scientific understanding of LOF is readily available in the literature, it would be useful to a) insert it into standards and b) research the influence of melt pool dimensional variance. Variance can blur the boundary of the process window. A small number of test prints should suffice to establish this boundary.
	2. Residual stress [57]	Peer-reviewed articles and public benchmarks (AM Bench) compare experimental measurements with simulations; but most are only visual. It is common to infer residual stress indirectly from cutting methods.	Inherent strain family of techniques are efficient (and implemented in commercial codes) but range of applicability is unknown. Fully coupled thermomechanical models are more predictive, but are more expensive, require expert users, and reliable input data.	Fully documented and peer-reviewed datasets that describe printing conditions and stress/strain measurements. Ideally using methods such as X-ray and neutron diffraction.	Improve predictive accuracy and reliability of simplified techniques (e.g., inherent strain) and improvement of the efficiency of more complex thermomechanical models.
	3. Distortion [57]	Peer-reviewed articles describe comparisons of distortion simulation with experimental measurements; however, agreement is not considered to be good in all respects.	More challenging than achieving a prediction of only the residual stress. Additional distortion during downstream processing (e.g., build plate removal, heat treatment) is also of interest.	Fully documented and peer-reviewed datasets that describe printing conditions and measurements of distortion – note the sensitivity of distortion to material properties via relaxation via plastic deformation.	Part distortion during printing is sensitive to boundary conditions, i.e., the mechanical constraints on the part combined with the thermal shrinkage. Therefore, validation and UQ of codes to predict distortion are complicated by the large variation in part geometries. Bring down uncertainty in distortion prediction by curating and re-analyzing data from different projects on distortion to build up confidence in this area over time.

Thematic Area	Topic	Current Status	Development Difficulty	Required Input and Validation Data, and Associated Challenges	Examples of Investment Opportunities
Physics – Process (cont.)	4. Full- part thermal history [212,213]	Examples using simplified numerical or semi-analytical approaches. Necessary to maximize computational efficiency. Accuracy of specific data for microstructure or flaw formation unclear.	Simplified models can be efficient and scalable, but lack in physical fidelity, often simplifying boundary conditions or material properties. Numerical models lack efficiency to scale to full parts.	Validation datasets based on thermography and thermocouple (T/C) measurements. Thermocouples offer good temperature measurement at a small number of locations, which cannot be considered full-field, i.e., T/Cs provide a small number of accurate T-t histories that help to calibrate surface thermography. Thermography provides surface temperature measurement but calibration is challenging. 3D measurements are infeasible.	Robust calibration approaches are needed that acknowledge the constraint of limited locations for T-t measurement. Explore the inverse problem of inferring process conditions from T-t history. Also need to develop multiscale methods so that one can zoom in to regions of particular interest (e.g., T/C locations, off-norm T-t histories). Opportunities for ML and reduced-order models. Reduce uncertainty by using validated full-field simulations as ground truth for reduced-order models.
	5. Build-chamber-scale effects (build thermal history/gas flow etc.)	Can use existing CFD techniques for chamber scale gas flow, but not many examples in the literature. Part-to-part thermal interactions, or interactions between gas flow distributions and deposition, are not well understood.	Challenging due to large length scales and necessary multi-physics coupling. Multiple model types likely needed for various purposes.	Gas flow data throughout build chamber with, for example, hot wire anemometer, can also use Schlieren optics (though quantification is more difficult). Part level data (temperature, microstructure, residual stress) for builds with different multi-part layouts.	Understanding effects of gas flow on thermal distributions and variability across the build plate. Interaction effects of multiple geometries in the same build on global scan behavior and subsequent effects on phase transformations, residual stress, and distortion.
	6. Keyhole and entrapped gas porosity [79]	Full-physics simulations are the gold standard but expensive. In the near-term, there is evidence that physics-inspired ML models can be validated for specific materials and printers.	Requires consideration for free surface evolution, effects of temperature on surface tension and vaporization, as well as keyhole stability and fluctuations that cause pore formation.	Material property data is not always well known. Likely also to be affected by heat source interactions and powder distribution. Validation requires direct observation of keyhole formation, but also requires understanding in complex processing conditions (e.g., scan path and geometry).	Studying fundamental mechanics of keyhole formation and stability, particularly in the presence of powder layers, multiple layer passes, denudation, etc. Machine learning using combinations of experimental and modeling data may be viable approach.
	7. Spatter prediction and induced flaws	Some examples of high-fidelity simulation that can capture some spatter effects, but little study on the effects of spatter on subsequent deposition steps.	Highly challenging, as it requires consideration of complex multi-physics interactions at the melt pool scale.	In process spatter observations at very high resolutions and speeds. Direct spatial correlation with effects on subsequent build quality.	Study of the nature of spatter formation and subsequent effects.

Thematic Area	Topic	Current Status	Development Difficulty	Required Input and Validation Data, and Associated Challenges	Examples of Investment Opportunities
Physics – Process (cont.)	8. Melt pool dynamics (e.g., fluid flow, keyholing) [214,215]	Many examples for various levels of model fidelity. Modeling approach varies strongly on the QOI for prediction.	Challenge depends on the model complexity, and the required balance of physical fidelity and computational expense. Many such models with different trade-offs may be formulated, spanning many orders of magnitude in expense.	Direct comparisons of fluid flow in melt pools of metals are challenging and have only been made on a qualitative basis.	Predicting keyhole stability based on high-fidelity models, and help to produce simplified relationships that may be used for practical application to larger build scales. Opportunity to couple multiple model scales, perhaps with AI/ML techniques.
	9. Solidification conditions [214]	Frequently extracted from melt pool models to give distributions of thermal gradient and solidification rate. However, very sensitive to melt pool shapes, and less frequently applied over larger scales or coupled to microstructure models.	Achieving accurate melt pool shapes is challenging, especially when conditions diverge from the conduction dominated regime. Achieving accurate predictions is critical for downstream microstructure prediction. It is also necessary to account for melt pool evolution over many scans/layers.	Input parameters can be uncertain, especially surface tension as a function of temperature. Validation through comparison with melt pool profiles. Ideally including both in-situ and post-mortem data.	Approaches for improved efficiency to capture larger length scale effects. For example, physics-driven approaches for effective heat source shapes that can help neglect explicit effects of fluid flow or keyholing.
	10. Melt pool variability	Simulation of melt pool variability requires full physics simulations. Both commercial and research codes exist. However, no evidence of use for understanding the observed statistical fluctuations, e.g., [75].	Highly challenging, because modeling this effect likely requires both high fidelity, and simulation over long length and time scales.	Validation will require careful statistical characterization of melt pool fluctuations and variability. Likely with in-situ characterization, either in conventional processing, or specialized instruments (e.g., synchrotron). Time- and direction-resolved laser reflection measurements may be useful.	Application of noise to continuum scale melt pool models to estimate fluctuations in melt pool dimensions. Study of natural fluctuations in the process to aid in accurate simulation of these sources of variation.
	11. Gas flow, plume, and laser interactions [216]	CFD modeling of the gas flows in PBF-LB systems is being reported by many groups. ML is being applied to, e.g., establish correlations between gas flow and spatter landing areas. Some measurements of gas-plume interaction and resulting melt pool shape are available [68,70].	Plume dynamics relative to heat source trajectory is expected to be important. Interactions with heat source behavior is a challenging area of research requiring very high-fidelity models with complex physical effects.	High-quality information on laser profiles will be necessary, as well as information on cover gas flow. In-situ measurement of laser interactions with the plume are expected to be highly challenging.	Study the effect of the orientation and geometry of the melt pool and plume relative to the gas flow and the laser incident angle. Seek to understand the variations in heat source interactions and the consequences for melt pool behavior and spatter formation.

Thematic Area	Topic	Current Status	Development Difficulty	Required Input and Validation Data, and Associated Challenges	Examples of Investment Opportunities
Physics – Process (cont.)	12. Powder flow and effects [217]	DEM codes exist but are limited in their fidelity with respect to particle shape. Subsequent interaction with the melt pool is sometimes considered using powder resolved models.	Consideration for granular flow, and especially motion of powder particles in response to gas dynamics in vicinity of heat source.	Quantitative measurements of particle motion during spreading. Effective powder densities for realistic spreading scenarios. Study of the effects of variations on powder characteristics and amount of powder recycling.	Models to identify the limits of powder characteristics that enable suitable flow properties to help guide reduction of feedstock cost.
	13. Powder recycling	Primarily experimental studies, and very alloy and process dependent. Few techniques available to estimate effects of processing on powder chemistry/quality, or downstream effects on subsequent processing.	No known computational approaches for modeling changes in powder characteristics during recycling. Likely needs to be linked to other models (e.g., DEM, or microstructrue evolution)	Powder composition and morphological characteristics through multiple recycling steps. Accurate measurement of atmosphere composition.	Identify effects of powder recycling on flowability and chemistry. Identify how these limitations may affect recycling practices, particularly for different materials, as some will be more sensitive than others. Good target for standards and best practice guides.
	14. Dissolved gas porosity [218]	Some analytical approaches, primarily adapted from casting and welding literature [218]. Challenging to apply and validate.	Requires modeling of gas solubility and precipitation, and inclusion of mushy zone effects.	Measurement of size and location of gas pores, particularly in cases where keyhole and LOF flaws have been adequently minimized.	Identify processing and alloying changes that may minimize the effect of gas porosity (e.g., hydrogen precipitation in Al alloys). Can be used to maximize mechanical performance, especially fatigue resistance.
	15. Surface roughness [219]	Very few examples of computational approaches, not well validated. Limited measurement data.	Very challenging to consider the partial melting and subsequent dynamics at the interface between part and powder bed. Explicit consideration for liquid-gas interactions are likely required.	Measurement of surface roughness with quantitative means for various surface orientations and process parameters. May also want to consider differences in feedstock characteristics.	Improve/decrease surface roughness to increase fatigue resistance in cases where post-machining is not possible.
Physics – Microstructure	16. Computational Thermodynamics [220]	For phase composition in cases where extensive thermodynamic databases exist such as low-alloy steels, stainless steels, commercial Al-alloys and Ni-alloys. For Ti alloys outside the standard set (e.g., with larger interstitial contents), however, the available databases are generally incomplete.	Techniques are known, well established, and available in commercial products. Major challenge lies in adapting to non-equilibrium AM cases (likely requires extension of existing databases) and quantifying uncertainty.	Measurements of phase stability at specific temperatures and compositions. May require measurement of metastable states in as-fabricated microstructures for many alloy systems.	Government-industry collaboration (following the AIM or ChiMaD models, for example) to develop thermodynamic data in a form that any CALPHAD package can input (or use for calibration). Focus on alloys modified for AM and new alloys in key areas, e.g., refractory alloys. Add UQ analysis to existing packages which is not yet available.

Thematic Area	Topic	Current Status	Development Difficulty	Required Input and Validation Data, and Associated Challenges	Examples of Investment Opportunities
Physics – Microstructure (cont.)	17. Thermo-kinetics	Available for kinetics of standard (Fe, Al, Ni) alloys processed via legacy methods. Gaps in terms of kinetics of standard alloys processed via AM.	Some kinetic databases exist but not all important parameters are always known. Initial and boundary conditions for diffusion calculations are challenging to establish.	Measurement of diffusional data. Study of phase transformations, possibly using in-situ techniques.	Extend kinetics models, especially diffusion to compositions used in metals AM. Extend diffusion models in particular to include complex interactions. Add UQ to the parts of CALPHAD packages that include kinetic data.
Physics – Microstructure (cont.)	18. Grain-scale microstructure [110,221,222]	Various types of CA and KMC with mostly qualitative comparisons with experimental data have been published. PF models have mostly concentrated at the dendrite scale with even more limited validation.	Models are very sensitive to input thermal conditions, and to parameters such as nucleation and interface response function. Currently do not account for mechanics of grain deformation during cooling and effects on texture development.	Quantitative measurement of grain characteristics, including texture, with associated highly pedigreed data for process conditions and melt pool behavior.	Full 3D simulations that include crystallographic texture are expensive. Even here, basic validation is needed against, e.g., AM Bench. To solve industry problems, reduced-order (fast-running) models are required. Need to emphasize R&D to take from purely qualitative to quantitative to predictive.
Physics – Microstructure (cont.)	19. Sub-grain microstructure [223,224]	PF is a commonly applied method. It is not clear, however, that any PF code has been subjected to software readiness development.	Challenging to extend models (e.g., PF) to complex, 3D multi-component alloy systems of industrial interest.	Precise measurement of spatial distributions of solute, especially as a function of local thermal conditions at various positions within melt pools.	Predict levels of segregation that may affect subsequent phase transformations or deformation characteristics. Extend existing models to larger numbers of alloying elements common for industrially relevant alloys.
Physics – Microstructure (cont.)	20. Dislocation structure	Discrete Dislocation Dynamics (DDD) is commonly used because MD is far more expensive. It is not clear that any DDD code has been subjected to evaluation of its software readiness level.	Highly challenging. Requires extension of DDD or other methods, and utilization of highly challenging characterization techniques.	Measurement of dislocation structure (e.g., TEM), and measurement of changes in grain orientation along build height (e.g., 3D EBSD).	Scientific understanding of the origin of dislocation structures is needed to validate computational models such as DDD.
Physics – Microstructure (cont.)	21. In-process cracking [225]	Abundant experimental work in the welding literature but little modeling. Some work in related fields such as casting [225].	Highly challenging because it requires simultaneous consideration of part scale stress evolution and local microstructure features.	Fractography associated with particular types of cracks, and correlation with both processing conditions and microstructure.	Identify specific classes of cracking that extend classification hierarchies that currently exist for casting and welding. Develop techniques to aid in alloy design and process optimization.

Thematic Area	Topic	Current Status	Development Difficulty	Required Input and Validation Data, and Associated Challenges	Examples of Investment Opportunities
Physics – Properties and Performance	22. Static mechanical properties (YS, work hardening) [226]	A small number of companies practice precipitate structure prediction (basically via CALPHAD tools) for the purposes of predicting mechanical properties. YS is reliably predicted in alloys with well-characterized thermo-kinetics. Work hardening is much harder to predict (and strongly temperature dependent).	Volume-averaged strengthening models can be highly effective if microstructural information is accurate. Determination of microstructure features is largest barrier, except where heterogeneous/anisotropic effects are concerned. However, most constitutive models are merely curve-fitting a preferred equation to limited data (e.g., single temperature or strain rate).	Validation of both precipitate and dislocation predictions against measured properties. For specific alloys, literature exists to document the effectiveness of YS modeling.	Some commercial solutions exist in this space, particularly crystal-plasticity FEA (CPFEA). Nevertheless, additional research to fill in gaps will be beneficial, e.g., to develop crystal-plasticity spectral methods (e.g., MASSIF, DAMASK). The main gap is a lack of generalization of current simulation packages that tend to be alloy-specific.
	23. Static mechanical properties	The situation is similar to that of basic mechanical properties but with additional complexity from the accumulation of damage leading to fracture.	Will require adaptation or extension of fracture models. In complex situations, will require detailed crystal plasticity or other numerical techniques.	Detailed experimental data, including fractography and microstructure correlations to mechanical testing. Will be alloy-specific in most cases.	Estimation of ductility for specific alloy classes to enable optimization of processing or modification to alloy composition.
	24. Creep	Plenty of examples of experimental work on creep of AM alloys (e.g., [260]), but few models aside from conventional power-law fitting of experimental data.	Very challenging, as active creep mechanisms will depend on specific microstructural features and application load cases. Complex microstructures in AM alloys are significant challenge, even for interpretation of experimental data.	Detailed creep studies, possibly including in-situ techniques such as DIC or X-ray/neutron diffraction. Correlation with microstructure features is critical.	Development of a fundamental understanding of creep behavior of AM microstructures. Application to optimize process conditions and design new creep-resistant alloys.
	25. Fatigue life (initiation and short crack growth)	Probabilistic models based on microstructure variability and flaw distributions. Underlying physics-based microstructural crack nucleation models are not sufficiently mature.	In order for probabilistic models to be effective, accurate knowledge of flaw populations, microstructures, and material properties are required. Challenges include accounting for these material characteristics and addressing material variability. Microstructure homogenization is not effective.	Very expensive to acquire sufficient measurement data. Properly measuring types (pore, particle, roughness), sizes, shapes, and locations of features that may lead to fatigue failure is critical. Microstructural features that may lead to fatigue failure are even more difficult to characterize.	Further maturation of physics-based microstructural crack nucleation models. Development of physics-informed ML models for fatigue life prediction. Incorporate in-process monitoring to characterize flaw populations.

Thematic Area	Topic	Current Status	Development Difficulty	Required Input and Validation Data, and Associated Challenges	Examples of Investment Opportunities
Physics – Properties and Performance (cont.)	26. Fatigue life (long crack growth) [234,235]	Most prevalent approach is to use empirical data and commercial software to perform numerical integration combined with geometry-specific fracture mechanics solutions. More complex 3D fracture mechanics tools also exist. Fundamental microstructure-based solutions are not available.	There is little incentive for development of fundamental microstructure-based solutions and achieving accuracy comparable to the empirical approaches is unlikely. Accounting for more complex crack growth phenomena such as crack interactions and fracture of heterogeneous and/or anisotropic media is non-trivial.	High-fidelity crack growth rate data are needed for continuum mechanics-based models. The lack of a fundamental basis greatly limits extensibility to different materials or conditions, leading to expensive testing requirements.	Accounting for more complex crack growth phenomena such as crack interactions and fracture of heterogeneous and/or anisotropic media.
	27. Fracture Toughness	Many experiments measuring toughness exist, but limited work in the literature on predicting material toughness. In general, it can be predicted from a simulation of the impact test itself. However, most simulation efforts are focused on predicting fracture toughness like K_{Ic}.	While the material toughness is related to the (quasi-static) stress-strain curve, there is not a clear relationship between the two. Modeling fracture surface contact and material non-linearity are complex and computationally intensive. Some advanced alloys exhibit additional deformation mechanisms (e.g., TRIP/TWIP), which can be challenging to capture with traditional continuum constitutive modelling.	Detailed characterization of chemical composition and microstructural evolution during deformation may be required. If using FEA methods, both static and dynamic material properties must be measured, possibly including temperature dependence.	Elucidating the role of anisotropy and heterogeneity on fracture toughness. Accounting for variable stress/strain conditions for parts with complex geometry. Designing tough AM materials, as well as heat treatments that result in strong and ductile behavior, is important in many structural applications.
	28. Environmental effects	Some work in the literature on experimental study of corrosion, few applications of modeling tools.	Unknown how important microstructural features of AM parts will be.	Detailed characterization of AM materials and relationship of environmental effects with respect to specific AM microstructure features. Quantitative measurement (e.g., EIS for corrosion) where possible.	Anticipate environmental effects will be critical for future applications. Will require models that help to predict effects of composition, processing, and microstructure.
	29. Part-scale geometric effects [236]	Some examples of modeling tools to estimate variation in e.g., melt pool dynamics, mostly using simplified models.	Largest challenge is to combine scalable modeling approaches with appropriate consideration for non-linear effects, such as temperature-dependent properties or complex boundary conditions.	Transient melt pool response for specific geometries and scan paths, and thermal data at various locations throughout processing.	Could use simplified estimation of geometric effects to trigger targeted application of more expensive high-fidelity models.

Thematic Area	Topic	Current Status	Development Difficulty	Required Input and Validation Data, and Associated Challenges	Examples of Investment Opportunities
Software Infrastructure	30. Non-intrusive UQ [203,204]	A variety of open-source and some commercial packages are available. Frequently used by academics but not widely adopted by industry.	Can primarily rely on existing software packages. Primary challenges lie in coupling models where necessary, and properly quantifying input uncertainty distributions.	Measurement uncertainties for physical input quantities.	Demonstration of rigorous UQ for AM models that are specifically relevant to Q&C practices.
	31. Intrusive UQ	Not available outside of a small number of niche academic codes.			
	32. Model validation	Quantitative techniques broadly understood, but not always applied.	Development required for validating complex multi-length scale and multi-time scale simulations. Another challenge is in community adoption.	Clearly defined metrics and thresholds need to be established for specific sets of model predictions and applications. Corresponding experimental data will be required.	Demonstration of quantitative model validation specifically for AM simulations, with direct application to Q&C practices. AM Bench is good example.
	33. Model coupling infrastructure	Some tools available.	Challenging to incorporate particular models and manage corresponding inputs/outputs. Requires high flexibility in software design as each application will require specific modeling tools.	Requires validation data across various coupled models individually, and collectively (hierarchical model validation).	Demonstrate integration of multiple models including validation data and quantitative UQ estimates.
Software – Accelerated Computation	34. ML/surrogate models [237]	A variety of open-source and commercial 3rd party software, but not natively supported for most physics-based codes.	Selection of ML or surrogate model architectures is often dependent on a specific application. Few users understand both ML/surrogate model methods and the physics applications. Obtaining appropriate training data is frequently challenging and/or expensive.	Large quantities of pedigreed and labeled experimental data may be required, depending on the application of interest.	Jointly define ML architecture and data collection/labeling strategies to target a critical Q&C relevant application.
	35. Physics-based reduced-order models	Approaches exist and are increasingly used, but not always readily available.	Requires detailed understanding of underlying models and mathematical techniques. Appropriate computational design (often application-driven) for maximizing efficiency is also necessary.	Reduced-order models require, at a minimum, validation against full-fidelity models for appropriate test cases.	Application of simplified thermal process models to understand effects of geometry and scan path.

Thematic Area	Topic	Current Status	Development Difficulty	Required Input and Validation Data, and Associated Challenges	Examples of Investment Opportunities
Software – Accelerated Computation (cont.)	36. Hybrid ML/Physics models	Some preliminary academic work, but nothing commercialized.	Open questions on architecture of hybrid approaches, with many possible options, but few realized. Will necessarily require significant amounts of both experimental and simulation data.	Experimental and simulation training and validation data. Type and quantity depend on application.	Incorporation of process sensing data and process modeling to predict flaws.

Appendix VII Glossary

The following definitions of key terms have been defined or adapted from the cited sources for the purposes of the present work.

Accuracy: The closeness of a parameter or variable (or a set of parameters or variables) within a model, simulation, or experiment to the true value or the assumed true value [187]

Additive Manufacturing (AM): Process of joining materials to make parts from 3D model data, usually layer upon layer, as opposed to subtractive manufacturing and formative manufacturing methodologies [261]

Allowable: A value derived from the statistical reduction of data from a stable process. The amount of data required to derive these values is governed by the statistical significance or *basis*. Application of allowables may require additional considerations for use in design [262].

Application Domain: Indicates the range of physical conditions where predictions are needed from the model for the application of interest; the domain that comprises the physical conditions for the real/physical system of interest; the application domain is commonly specified in terms of the range of values of all input parameters of the model; uncertainties in the application domain are not necessarily related to uncertainties that exist in laboratory experiments [166].

Benchmark Measurement Data: Formalized measurement datasets with measurement uncertainties produced and distributed with the intent to provide real-world measurement data for guiding and validating computational models

Calibration: The process of adjusting numerical or modeling parameters within the model to improve agreement with a referent. Note: Calibration can also be known as *tuning* [187] . Calibration can also refer to a procedure designed to check or set settings on measuring instruments or other precision equipment. An example is calibrating the laser power for a PBF-LB machine.

Certification: A documented assurance that the product being delivered meets all applicable requirements

Confidence: Difference between an estimated statistic of a set of samples, e.g., the mean, and the true value of the statistic [166]

Computational Materials (CM): The broad range of approaches for simulation of material processing, material structure, and/or material properties

Credibility: The trust, established through the collection of evidence, in the predictive capability of a computational model for a context of use [263]

Credibility Assurance Framework: A structured methodology or process used to verify credibility of a computational model

Defect: A flaw whose size, shape, orientation or location makes it detrimental to the useful service of its host object or exceeds an accept/reject criterion of an applicable specification. Not all flaws exceed an accept/reject criterion and are therefore not defects. Defects typically require some form of corrective action [264]. (see also: *Flaw*)

Delta Qualification: Re-qualification necessary when processing conditions or manufacturing process steps of a fixed-process have been modified. Conditions could include machine state, configuration, model, operating software, material/material supplier, or process parameters.

Economies of Scope: Efficiencies formed by part variety with heightened flexibility, shorter production runs, more customized products, faster responses to changes in market demand, and greater control and accuracy of processes [265].

FAIR data management: Broadly accepted guidelines for enhancing the reusability of data holdings. The four foundational principles are Findability, Accessibility, Interoperability, and Reusability.

Fidelity: The amount of detail with which a model describes an actual process. Relevant features might include the descriptions of geometry, model symmetries, dimensionality, or physical processes in the model. High-fidelity models attempt to capture more of these features than do low-fidelity models [266].

Flaw: Interruption, imperfection, or irregularity in the physical structure or material state of a part or a specimen [264] (see also: *Defect*).

Hierarchical Benchmarks: A series of coupled benchmark measurements that spans a complete process

Integrated Computational Materials Engineering (ICME): A discipline coupling CM tools to accelerate materials development and unify design and manufacturing [10]

Measurement: An experimental process that produces a value that can reasonably be attributed to a quantitative property of a phenomenon, body, or substance

Model: A conceptual, mathematical, or computational representation of a system, process, or phenomena

Model, Machine Learning: A model that has been developed via the operation of a numerical algorithm, which is expressed in terms of hyperparameters, architecture, and coefficients, and which is not necessarily physics-based; for example, a regressor or classification neural net model that takes images as input and quantifies the information contained therein.

Precision: The implied degree of certainty with which a value is stated, as reflected in the number of significant digits used to express the value—the more digits, the more precision [266]

Prediction: Use of a model to foretell the state of a physical system under conditions for which the model has not been validated

Process-Intensive Material (PIM): Materials created through manufacturing processes where properties can be highly sensitive to multiple interacting parameters. It is the degree of sensitivity, complexity, and need for enhanced process-control that determine a process's intensiveness.

Qualification: An evidence-based procedure to confirm compliance with applicable key characteristics as required by a product standard or technical specification(s)

Quantity of Interest (QOI): A numerical characteristic of the system being modeled that is of interest to stakeholders, typically because it informs a decision. To be useful, the model must be able to provide, as output, values of or probability statements about QOIs [266].

Simulation: A specific instantiation of a computational model with one set of input parameters that outputs quantities of interest

Sub-models: Computational models of restricted scope that are used to provide critical inputs to the application computational model that is being assessed

Surrogate Models: A relatively simplified model relating the inputs and outputs of a more complex model or simulation, as opposed to real-world observations (e.g., measurements)

Uncertainty, Aleatoric-: A measure of the uncertainty of an unknown event whose occurrence is governed by some random physical phenomena that are either (1) predictable, in principle, with sufficient information (e.g., tossing a die), or (2) essentially unpredictable (radioactive decay) [266]

Uncertainty, Epistemic-: A representation of uncertainty about propositions due to incomplete knowledge. Such propositions may be about either past or future events [266].

Uncertainty, Measurement-: A non-negative parameter characterizing the dispersion of the quantity values attributed to a measurand, including both systematic and definitional effects. Evaluation may be accomplished through use of either statistical (Type A) or alternate methods (Type B, e.g. certified reference materials, calibration, etc.) [139].

Uncertainty, Simulation-: Imperfectly known information concerning an object or issue; potential deficiency in any phase or activity of the modeling and simulation process that is due to inherent variability (aleatoric or irreducible uncertainty) or lack of knowledge (epistemic or reducible uncertainty) [166]

Uncertainty Quantification: The process of numerically describing uncertainty in input data as well as computed and empirical QOIs, with the goals of accounting for all sources of uncertainty and quantifying the contributions of specific sources to the overall uncertainty

Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model [266]

Validation Domain: The region enclosing all sets of model inputs for which the model responses compare favorably with the referent [187]

Validation Metric: The statistical methodology for quantifying the degree of agreement between computational and experimental results for the intended use of the model

Verification: The process of determining the extent to which a model or simulation is compliant with its requirements and specifications as detailed in its conceptual models, mathematical models, or other constructs [187]

Verification Domain: The region enclosing all sets of model inputs for which the solution is determined to be correct and satisfy requirements for computational accuracy [187]

Verification, Solution-: The process of determining as completely as possible the accuracy with which the algorithms solve the mathematical-model equations for a specified QOI [266]

Appendix VIII Acronyms

AFRL	Air Force Research Laboratory
AI	Artificial Intelligence
AIAA	American Institute of Aeronautics and Astronautics
AM	Additive Manufacturing
AM Bench	Additive Manufacturing Benchmark Test Series
AMS-AM	SAE International Aerospace Material Specifications for Additive Manufacturing
AMSC	Additive Manufacturing Standards Collaborative
APT	Atom Probe Tomography
ARL	Army Research Laboratory
ASME	American Society of Mechanical Engineers
CA	Cellular Automata
CAD	Computer Aided Design
CAF	Credibility Assurance Framework
CALPHAD	Computer Coupling of Phase Diagrams and Thermochemistry (used to be CALculation of Phase Diagrams)
CCT	Continuous Cooling Transformation
CEN	European Committee for Standardization
CFD	Computational Fluid Dynamics
CM	Computational Materials
CM4QC	Computational Materials for Qualification and Certification
COS	Commercial Open-Source
COTS	Commercial Off-the-Shelf
CP	Crystal Plasticity
CPFEA	Crystal Plasticity Finite Element Analysis
CPU	Central Processing Unit
CT	Computed Tomography
DARPA	Defense Advanced Research Projects Agency
DEM	Discrete Element Method
DfM	Design for Manufacturability
DFT	Density Functional Theory
DIC	Digital Image Correlation
DMREF	Designing Materials to Engineer and Revolutionize our Future
DOD	Department of Defense
DOE	Department of Energy
DoE	Design of Experiments
DREAM3D	Digital Representation Environment for Analysis of Materials in 3D
DSC	Differential Scanning Calorimetry
DT	Digital Twin
DXR	Dynamic X-ray Radiography
EBSD	Electron BackScatter Diffraction
ECI	Eddy Current Inspection
ECP	Exascale Computing Project
EDD	Energy Dispersive Diffraction
EIDP	End-Item Data Package
EIS	Electrochemical Impedance Spectroscopy

ENSIP	Engine Structural Integrity Program
F&DT	Fatigue and Damage Tolerance
FAIR	Findable, Accessible, Interoperable, Reusable
FAA	Federal Aviation Administration
FDA	Food and Drug Administration
FEA	Finite Element Analysis
FEP	Foundational Engineering Problem
FOS	Free Open-Source
FPI	Fluorescent Penetrant Inspection
GOTS	Government Off-the-Shelf
GPU	Graphical Processing Unit
HAZ	Heat-Affected Zone
HEDM	High-Energy Diffraction Microscopy
HPC	High-Performance Computing
ICME	Integrated Computational Materials Engineering
IEEE	Institute of Electrical and Electronics Engineers
IMQCAM	Institute for Model-based Qualification and Certification of Additive Manufacturing
IPAMS	Integrated Platform for Additive Manufacturing Simulations
IR	Infrared
IS	Importance Sampling
ISO	International Organization for Standardization
IT	Information Technology
KMC	Kinetic Monte Carlo
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
LANL	Los Alamos National Laboratory
LIFT	Lightweight Innovations for Tomorrow
LOF	Lack of Fusion
MD	Molecular Dynamics
MGI	Materials Genome Initiative
MIP	Materials Innovation Platform
ML	Machine Learning
MML	Materials Maturity Level
MMPDS	Metallic Materials Properties Development and Standardization
MOOSE	Multiphysics Object Oriented Simulation Environment
MRL	Manufacturing Readiness Level
NAS	National Academy of Sciences
NASA	National Aeronautics and Space Administration
NAVAIR	Naval Air Systems Command
NAVSEA	Naval Sea Systems Command
NDE	Nondestructive Evaluation
NDI	Nondestructive Inspection
NDT	Nondestructive Testing
NIST	National Institute of Standards and Technology
NSF	National Science Foundation
OEM	Original Equipment Manufacturer
ONR	Office of Naval Research
ORNL	Oak Ridge National Laboratory
OSTP	Office of Science and Technology Policy

PBF-LB	Powder Bed Fusion – Laser Beam
PDE	Partial Differential Equation
PETS	Process Equivalent Test Specimen
PIM	Process-Intensive Material
PIML	Physics-Informed Machine Learning
PF	Phase Field
PRISMS	Prediction of Realistic Integrated Structure Materials Science
PSPP	Process Structure Property Performance
Q&C	Qualification and Certification
QOI	Quantity of Interest
R&D	Research and Development
RAM	Random Access Memory
ROI	Return on Investment
RVE	Representative Volume Element
SAE	Society of Automotive Engineers
SDO	Standards Development Organization
SeCAV	Sequential Calibration and Validation
SEM	Scanning Electron Microscopy
SME	Subject Matter Expert
SML	Simulation Maturity Level
SPPARKS	Stochastic Parallel PARticle Kinetic Simulator
SURGE	Structures Uniquely Resolved to Guarantee Endurance
TEM	Transmission Electron Microscopy
TIM	Technical Interchange Meeting
TRL	Technology Readiness Level
TRIP	Transformation-Induced Plasticity
TTT	Time-Temperature Transformation
TWIP	Twinning-Induced Plasticity
UQ	Uncertainty Quantification
USAF	United States Air Force
V&V	Verification and Validation
VVUQ	Verification, Validation, and Uncertainty Quantification
WG	Working Group
YS	Yield Strength

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