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

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Nomenclature

ACP	NASA Advanced Composites Project
AFRL	Air Force Research Laboratory
AM	Additive Manufacturing
ARMD	NASA Aeronautics Research Mission Directorate
ASCI	Accelerated Strategic Computing Initiative
ASME	American Society of Mechanical Engineers
CFD	Computational Fluid Dynamics
COE	Center of Excellence
EASA	European Union Aviation Safety Agency
FAA	Federal Aviation Administration
ICME	Integrated Computational Materials Engineering
JSSG	Joint Service Specification Guide
L-PBF	Laser-Powder Bed Fusion
LLNL	Lawrence Livermore National Laboratory
ML	Machine Learning
MMPDS	Metallic Materials Properties Development and Standardization Handbook
MRL	Manufacturing Readiness Level
NASA	National Aeronautics and Space Administration
NIST	National Institute of Standards and Technology
NDE	Non-destructive Evaluation
OEM	Original Equipment Manufacturer
P-V	Power vs. Velocity
Q&C	Qualification and Certification
SOA	State-of-the-Art
SME	Subject Matter Expert
TIM	Technical Interchange Meeting
TRL	Technology Readiness Level
TMS	The Minerals, Metals and Materials Society
UQ	Uncertainty Quantification
V&V	Verification and Validation

Abstract

This report documents the goals, organization and outcomes of a Technical Interchange Meeting (TIM) on Computational Materials Approaches for Qualification by Analysis, co-organized by NASA, NIST and the FAA. The TIM was held at NASA Langley Research Center on January 15-16, 2020. Approximately 60 subject matter experts (SMEs) representing 8 aerospace manufacturers, 7 government organizations and 2 universities participated. Expertise of the SMEs spanned the Technology Readiness Level (TRL) scale from the low-to-mid TRL focus of government laboratories and universities to the high TRL perspective of the regulatory organizations and aerospace manufacturers. During this TIM, the future needs of the government regulators and manufacturers 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, 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 qualification and certification (Q&C). The TIM focused on process-intensive metallic materials technologies, including, but not limited to, additive manufacturing. Participation was roughly evenly divided among the processing and performance tracks, suggesting that both topic areas are generally perceived as being both valuable and requiring additional investment. The output of this TIM may be used by both participating and other organizations, in part, as guidance for future national efforts on maturing computational materials capabilities for use in the Q&C of advanced metallic material systems in aerospace applications.

1. Introduction

This report documents the goals, organization and outcomes of a TIM on Computational Materials Approaches for Qualification by Analysis, co-organized by NASA, NIST and the FAA. The TIM was held at NASA Langley Research Center on January 15-16, 2020. Approximately 60 SMEs representing 8 aerospace manufacturers, 7 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 regulatory organizations and aerospace manufacturers. During this TIM, the future needs of the government regulators and manufacturers motivated the overall discussion and framed the input given by the government laboratories and universities.

The TIM began with several plenary presentations on topics related to the state-of-the-art of computational materials, requirements and challenges for Q&C, and regulatory considerations and standards. Afterward, the group divided into two tracks related to i) Process to Microstructure relationships and ii) Microstructure to Performance relationships, that were aimed at answering nine questions from each of these distinct but complementary perspectives. Questions were developed by the TIM organizers to focus the conversation and spanned topics ranging from the identification of gaps in current capabilities for Q&C to forecasting capabilities that NASA and NIST should champion to enable next-generation Q&C of process intensive metallic materials.

The TIM was inspired by three related factors: 1) the aerospace industry's increasing interest in expanding the use of computational materials for Q&C of process-intensive metallic materials technologies in the aerospace industry, 2) the rapid maturation of computational materials capabilities across a range of applications and 3) a general lack of coordination of development and investment in these capabilities by funding organizations.

The key objectives of the TIM were to understand existing gaps in model-based, 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. The TIM focused on process-intensive metallic materials technologies, including, but not limited to, additive manufacturing (AM).

The TIM followed from NASA Aeronautics Research Mission Directorate's Materials and Methods for Rapid Manufacturing for Commercial and Urban Aviation Workshop that was held in Tyson's Corner, Virginia, on November 14-15, 2018 [1]. Topic areas of that workshop were much broader than those of the TIM and focused on identifying and assessing the state of technology areas, understanding critical technology gaps and identifying high-priority investment areas relevant to rapid/advanced manufacturing over a range of topics related to manufacturing of metallic and polymeric composite materials.

The TIM was the next step by the participating government agencies, industry and academia to better understand Q&C challenges while building and strengthening the enduring relationships needed to support the required capability development. The TIM was organized by Ed Glaessgen (NASA Langley); Lyle Levine, Alkan Donmez and Paul Witherell (NIST); and Michael Gorelik (FAA). Session chairs included Eddie Schwalbach (AFRL), Michael Gorelik (FAA), Tony Rollett (Carnegie Mellon University), Harry Millwater (University of Texas at San Antonio), Lyle Levine (NIST) and Corbett Battaile (Sandia National Laboratory). A complete set of notes for each session was recorded by research scientists at NASA Langley, including Andy Ramlatchan, Wes Tayon, Josh Fody, Sai Yeratapally, David Wagner and Andy Newman. Additionally, the attendees were welcomed by Jonathan Ransom, Langley's Deputy Director for Structures and Materials, and Mary DiJoseph, Langley's Aeronautics Research Director.

Several prior related publications address various related aspects of the use of modeling and simulation for Q&C. Among these are efforts sponsored by Sandia National Laboratory, Air Force Research Laboratory, The American Society of Mechanical Engineers (ASME), The Minerals, Metals and Materials Society (TMS), NASA, the FAA, and the European Union Aviation Safety Agency (EASA).

Oberkampf and co-workers developed the Predictive Capability Maturity Model (PCMM) that can be used to assess the level of maturity of computational modeling and simulation (M&S) efforts [2]. This model contains six areas that cover Representation and Geometric Fidelity, Physics and Material Model Fidelity, Code Verification, Solution Verification, Model Validation and Uncertainty Quantification and Sensitivity Analysis, with four increasing levels of maturity. Similarly, Cowles and co-workers developed two documents that provide a summary of a recommended approach to verification and validation (V&V) supporting Integrated Computational Materials Engineering (ICME) [3,4]. These descriptions of V&V planning checklists and a related ICME Tool Maturity Level assessment guide, help to provide guidance to the current effort.

Additionally, the ASME Standards Committee on Verification and Validation in Computational Solid Mechanics (V&V 10) has developed and released a V&V guide for solid mechanics that focuses on developing a verification and validation plan [5, 6]. The guide is available through ASME publications as V&V 10-2006. Additionally, ASME has a number of other V&V related publications such as ASME V&V 20 for computational fluid dynamics and heat transfer [7] and ASME V&V 40 for medical devices [8]. Two related reports have been published under the auspices of TMS discussing V&V of computational models associated with the mechanics of materials and accelerating the broad implementation of V&V in computational models of the mechanics of materials and structures [9, 10].

An encompassing vision for computational materials was recently published by NASA and includes identification of the critical technical and cultural challenges and gaps facing the computational materials community, in addition to key core technical work areas required to build the required collaborative digital environment [11]. Models and Methodologies, Multiscale Measurement and Characterization Tools and Methods, and Verification and Validation were included among the nine key areas.

Finally, the FAA has sponsored several workshops regarding quality and certification challenges for additively manufactured metal parts [12]. The objectives of the FAA workshops were to provide additional training and reference materials on AM processes to FAA employees, provide a comprehensive review of industry and OEM progress and challenges regarding AM applications, and promote collaboration both across government/academia/industry and within the FAA and EASA, regarding Q&C of metal AM parts. Breakout sessions focused on Design Data for Qualification and Certification, Fatigue and Fracture Considerations and Non-Destructive Evaluation (NDE) Inspection and In-situ Process Monitoring.

The remainder of this report is organized as follows: The plenary speakers, their affiliations and presentation titles are provided. Next, a description of each of the two tracks, the Processing to Microstructure track and the Microstructure to Performance track, is given along with the nine questions addressed in each track. A summary of the participants' collective responses to each of the nine questions is then presented with the workshop-identified potential investment areas (Question 9) included in their entirety. Finally, a summary of the workshop is provided. For completeness, Appendix A contains the complete program including a list of symposia session presentation titles and presenters, Appendix B contains a list of participating organizations, while Appendices C1 and C2 give the complete list of questions and responses for Track 1 – Process to Microstructure and Track 2 – Microstructure to Performance, respectively.

2. Plenary Speakers, Topic Areas and Summary of Observations

2.1. Plenary Speakers and Presentation Titles

This section briefly outlines the topics considered during the plenary and working sessions. The first group of presentations by Greg Olsen (QuesTek), Jim Belak (LLNL) and Michael Gorelik (FAA) focused on identification of the SOA of computational materials and predictive capabilities. The second group of presentations by Rick Barto (Lockheed Martin), Nate Ashmore (Boeing), Vasisht Venkatesh (Pratt and Whitney) and Jerry Nanni (Bell) provided perspectives from the aerospace industry related to the series of questions listed in Section 2.2. Finally, the third group of presentations by Doug Wells (NASA) and Michael Gorelik (FAA) offered regulatory considerations and standards. A summary of the plenary speakers, their affiliations and presentation titles are given in Table 1.

Table 1: Plenary Speakers and Presentation Titles

Session	
Speaker	***Presentation***
SOA of Computational Materials and Predictive Capabilities	
Greg Olsen – Chief Science Officer, QuesTek Innovations	SOA of Computational Materials
Jim Belak – Senior Scientist, Lawrence Livermore National Laboratory	Center for Materials in Extreme Environments
Michael Gorelik – Chief Scientist for Fatigue and Damage Tolerance, Federal Aviation Administration	Example of Industry Activities Toward Development of Predictive Durability Assessment
Perspectives from Leaders in the Aerospace Industry	
Rick Barto - Senior Manager Materials Solutions, Lockheed Martin	Lockheed Martin Perspectives
Nate Ashmore - Manager – Next Gen Metals Technology, Boeing Research and Technology	Boeing Perspectives
Vasisht Venkatesh - Associate Director, Materials Modeling & Methods, Pratt & Whitney	Pratt & Whitney Perspectives
Jerry Nanni - Manager, Manufacturing Innovation, Bell	Bell Perspectives
Regulatory Considerations and Standards	
Doug Wells – NASA Deputy Technical Fellow for Materials, NASA Marshall Spaceflight Center	NASA AM Standard
Michael Gorelik – Chief Scientist for Fatigue and Damage Tolerance, Federal Aviation Administration	Regulatory Considerations for Modeling and Simulation

2.2. Questions to the Participants

Two concurrent tracks focused on forecasting the future of various technologies related to computational materials approaches for model-enabled qualification followed the plenary session. The participants self-selected their attendance in either Track 1- Process to Microstructure or Track 2 – Microstructure to Performance to address a series of nine questions that were divided into three groups having similar themes. The roughly even participation in each of the tracks suggests that both topic areas are generally perceived as being both valuable and requiring additional investment.

The first eight questions were designed to take the participants through a logical progression, including:

- Identification of gaps in current capabilities for Q&C
- Consideration of the role that computational materials, V&V and data science can play in closing those gaps
- Opportunities for leveraging computational materials capabilities in other domains
- Ideas about sharing information and engagement of other organizations
- Balancing of simulation and experiment in a mature state of these capabilities

These eight questions led to the final question and overarching goal of the TIM: *determination of computational materials capabilities that NASA and NIST should champion to enable next-generation qualification of process intensive metallic materials.*

The questions to the participants, their groupings and the session facilitators are given below.

Group 1 questions - Qualification Gaps, SOA and Challenges
Facilitators: Track 1-Eddie Schwalbach, Track 2 – Michael Gorelik
Q1: What gaps cannot be addressed using traditional qualification methods or processes?
Q2: What is the current SOA for computational materials, including examples of success stories?
Q3: What are the main qualification challenges that may be addressed by computational materials-enabled capabilities?

Group 2 questions - Leveraging of Related Capabilities and Organizations
Facilitators: Track 1 – Tony Rollett, Track 2 – Harry Millwater
Q4: How can the current or near-term use of computational materials in non-qualification frameworks be leveraged to mature the capabilities for qualification, developing a pathway for leveraging?
Q5: Are there any competition insensitive ways to share information (pre-competitive)? Is there a pathway to leverage internal company capabilities for use by the larger community?
Q6: Is there a role that industry working groups/standards organizations could play in this process? Where do the standards opportunities lie?

Group 3 questions - Capability Development

Facilitators: Track 1 – Lyle Levine, Track 2 - Corbett Battaile

Q7: What is the role of V&V and Data Science in the maturation of computational materials capabilities?

Q8: What is the appropriate balance between modeling and testing for a fully mature computational materials framework (end state vision) to achieve the desired state for next-generation (computational materials-enabled) qualification?

Q9: What capabilities should NASA & NIST champion to enable next-generation qualification of process intensive metallic materials (e.g., AM). What is the timeline and phased approach at 5, 10, 20 years?

2.3. Summary of Responses for Each Track

The workshop resulted in numerous observations that may inform the participating organizations' decision making at various levels. Some highlights from the responses to each question are presented here with complete input from each session provided in Appendices C1 and C2.

Group 1 Summary - Qualification Gaps, SOA and Challenges

Process to Microstructure	**Microstructure to Performance**
***Question 1: What gaps cannot be addressed using traditional qualification methods or processes*?**	
• Understanding of process-microstructure relationships in materials produced by AM including prediction of microstructure, phases, defects and dislocation density. • Prediction of spatial variations in the above with respect to component geometry and location specific process variation. • Cost and time-effective development of material databases. • Effect of reuse of metallic powder on microstructure and properties. • Machine to machine variability.	• Variability and distribution of defects including rogue anomalies; effects of reuse of powder. • Determination of critical defect size; crack initiation. • Standardized models of underlying physics from micro-to-continuum scales. • Long-term performance under cyclic loading and service environments. • Determination of structural feature dimensions where continuum mechanics is no longer valid. • Effects of non-equilibrium microstructure, residual stress, etc. • Characterization/simulation of microstructurally short fatigue crack growth.
Question 2: What is the current SOA for computational materials, including examples of success stories?	
• Phase-field has been useful for understanding behaviors in general but is not sufficiently mature for application to real (many component) alloys. • Qualitative prediction of part-scale residual stresses. Accurate quantitative part-scale and all micro-scale predictions are beyond SOA. • High fidelity L-PBF process model from LLNL group to identify importance of various phenomena; but expensive and not tractable at part scale; needs careful multi-scaling. • Quantification of uncertainties is beyond SOA.	• Success stories include the ability to develop three-dimensional microstructure from experimental observations, crystal plasticity, probabilistic damage tolerance and development of reduced order models. • SOA for electronics (semiconductors) materials is mature, from ab initio → atomic → full scale. Use as an example for benchmarking of best practices. • Computational NDE and big data analytics is being adopted for research, with interest by OEMs. • Prediction of observable experimental results by showing results from sensitivity studies to aid in understanding of which inputs have the most influence on performance.

Question 3: What are the main qualification challenges that may be addressed by computational materials-enabled capabilities?	
• Development of data driven approaches that build linkages between in-situ monitoring data and location specific microstructure. • Prioritization of phenomena that most significantly contribute to uncertainties. • Missing critical thermo-physical data for materials models. • Use of computational materials to evaluate alloys and perform alloy design over the entire AM process window. • Computational tools to help understand machine to machine variability and perform sensitivity analysis. • Development of physics-driven and data-driven models for build quality (defect structure and microstructure in general) that are adaptable to the increasing understanding of AM processes.	• Reduction of cost, time and number of tests. • Uncertainty quantification and management. • Quantifying the effects of defects, critical initial flaw size and location-specific properties. • Leveraged use of computational materials to support quantitative condition-based maintenance. • Development of coupon-component transfer functions. • Parametric studies to control variables that are difficult to control experimentally. • Qualification and certification by analysis. • Transferring qualification from single part (design) to part family. • Transferring qualification from machine to machine.

Group 2 Summary - Leveraging of Related Capabilities and Organizations

Process to Microstructure	**Microstructure to Performance**
Question 4: How can the current or near-term use of computational materials in non-qualification frameworks be leveraged to mature the capabilities for qualification; developing a pathway for leveraging?	
• Support use of computational tools to support proposals for materials substitution to regulatory boards (FAA, Air Force, NASA, Navy, etc.). • Use of computational materials to predict Power-Velocity (P-V) maps; many process-to-structure relationships are in need of robust validation. • Matching parameters of importance from computational materials to available measurement capabilities (e.g., melt pool length and cooling rate of individual tracks, surface tension). • Help OEMs to improve the business case for expanding the application of AM. • Use of computational materials to suggest process parameters needed to manage surface roughness and defect characteristics. • Determining budgets for model uncertainty, process uncertainty and measurement uncertainty.	• Leverage NIST AM-Bench, AFRL Challenge Series, ASTM AM COE - known/trusted/validated data for comparison. • Communication needed between regulators and industry; develop roadmaps to determine future needs for toolsets; involvement of standardization organizations, ASTM, NIST, etc. • Tool maturation to bridge entire process-to-performance space is needed; in general, the volume of data/information is insufficient to support qualification although some success stories exist (e.g., landing-gear steels). • Use computational materials models in intermediate applications, e.g., to interpret in-situ monitoring. • Develop approaches for certification of general processes for classes of materials rather than specific parts/processes/materials.
Question 5: Are there any competition insensitive ways to share information (pre-competitive)? Is there a pathway to leverage internal company capabilities for use by the larger community?	
• Opportunities for sharing raw test data – the sensitivity for companies is the use of data for design allowables. • Possibility for sharing data from Metals Affordability Initiative (MAI) projects; the challenge is to obtain a release from all the participating companies.	• Success stories include the Advanced Composites Project NDE handbook that developed sharable NDE standards/data library, the FAA-sponsored Turbine Rotor Material Design, RISC working group where data was "pooled" and the Metals Affordability Initiative (MAI). • Developing formats and limited access repositories for sharing existing government-owned data, models and pre-competitive results; maintaining provenance.

Question 6: Is there a role that industry working groups/standards organizations could play in this process? Where do the standards opportunities lie?	
• Development of an industry-led Steering Group that could identify high priority issues. • Development of guidance for addressing the many regulatory bodies (e.g., DoD Airworthiness, JSSG-2006, MILT-STD -1530D, AWB-1015, FAA) to which companies must submit packages. Currently, such interactions (and packages) do not typically include computational materials. • A geometry-based approach to allowables is unlikely to work because of the complexities introduced by the manufacturing process. • The use of Process Equivalent Test Specimens (PETS) applies to all processes and technologies, not just AM, so this could represent an opportunity for advocacy by a Steering Group (and equivalent bodies).	• Interest in consortia of industry/federal groups to help standardization organizations - serve as a Steering Group to provide vision. • Communication needed between regulators and industry; develop roadmaps to determine future needs for toolsets; involvement of standardization organizations, ASTM, NIST, etc. • FAA is moving towards performance-based regulations (not prescriptive; moving away from defining means of compliance); going forward public standards will define means of compliance. • Calibration of codes/methods (standardization) could be addressed by government, e.g., NIST. • Need standards of application programming interface (API) for code access, and standardization of data between codes, e.g., schema (Success story: NDE sharable models working group). • Standards need to be expanded to support AM (e.g., O, N content allowables in alloys).

Group 3 Summary - Capability Development

Process to Microstructure	Microstructure to Performance
Question 7: What is the role of V&V and Data Science in the maturation of computational materials capabilities?	
• Improved coordination and communication between measurement teams (NIST, NASA, AM-Bench, etc.) and simulation teams would allow measurement priorities to better reflect OEM needs. • Prioritization of measurement needs must target factors that have a strong effect on the manufacturing processes, e.g., quantitative values and functions for the thermophysical parameters used as model input. • Procedures and standards for calibrating both the build parameters and the in-situ monitoring systems are critical for making build systems interchangeable. • Bridging the gap between measurements and microstructure would have a major impact on build quality; determination of which in-situ monitoring systems are best for a given purpose. • Provide systematic and consistent collection of metadata and data types. • Ensure a proper intersection between measurement outputs and modeling requirements.	• Uncertainty management in computational materials, including, calibration of material model parameters. • Increasing the ability to couple NDE data with computational materials models to determine effects of defects. • Development of supporting approaches needed to provide coverage over multi-dimensional parameter spaces. • Supporting a clear plan for generation of user data throughout the Q&C process, including model development and model calibration. • Determination of the domain over which codes can correctly be declared as being "validated." • Clear delineation of computational model V&V (and its implementation) separate from software V&V. • Development of industry-accepted data provenance protocols, common data models and API standards. • Development of a paradigm that attaches micro-structure constitutive models, instead of tables of coefficients, to Q&C activities/component properties.
Question 8: What is the appropriate balance between modeling and testing for a fully mature computational materials framework (end state vision) to achieve the desired state for next-generation (computational materials-enabled) qualification?	
• Lessons learned from other domains (e.g., wind tunnels and computational fluid dynamics) may help determine how far we can practically go in using	• The appropriate balance is dependent on intent, acceptable level of risk (e.g., component criticality),

simulations to replace some testing. The appropriate balance is also largely determined by those organizations responsible for certification. • Formal procedures and metrics for determining the appropriate testing for validation are needed. • Requires reconciliation between validation requirements from the simulation community and available capabilities for experimentation and measurement. • Needs reliable and extensible machine learning capabilities across different AM machines. • Development of alloys designed for AM processes would improve performance reproducibility and decrease machine-to-machine variability.	NDE and measurement capabilities, in addition to cost and time requirements. • Simulations and experiment are becoming increasingly interdependent; future determination of experimental requirements will follow simulation validation and calibration requirements and will continue to evolve as simulations mature. • Validation tests should be targeted to critical locations (system-wide assessment informs component test needs). • The Accelerated Strategic Computing Initiative (ASCI) could be used as a model. • Higher-level (component or family) testing and purpose-designed testing will increase in importance. • A hybrid approach should be considered: combine modeling and data analytics in an optimal way. Data generation should support more than just model development.
Question 9: What capabilities should NASA & NIST champion to enable next-generation qualification of process intensive metallic materials (e.g., AM). What is the timeline and phased approach at 5, 10, 20 years?	

All years:
• NIST (AM-Bench) and NASA can provide robust data for simulation V&V. Another source is DoD (e.g., AFRL Challenge Series).
• Think beyond direct physics-based approaches, i.e., consider how to integrate data driven approaches.
• Develop an understanding of the inherent sources of variability, including machines, processes and feed stock.
• Work with partner organizations to develop improved mechanisms and guidance for acquiring and sharing data and metadata.
 	
5 years:
• Provide prescription for measurements and calibrations to validate a basic set of process parameters. These should be used to qualify both process parameters and machines. Example: parameters for laser powder bed fusion include laser power, scan velocity, laser power distribution function, and hatch spacing.
• Make the connection between the set of process parameters and the local state of the material for a narrow set of materials and conditions. This goes beyond existing P-V maps that only deal with two process parameters.
• Develop a framework for defining and implementing model maturity levels, with specifications for V&V at each step.
• Although a given feedstock chemistry typically falls within formal alloy specifications, these specifications are often broad enough to introduce substantial variation in part performance. Work with standards organizations such as ASTM to address this problem of material specifications for AM feedstocks.
	All years:
	• There is a pervasive need for "computational-based design for inspectability" to be integrated into the design process.
	• Develop plans to highlight incremental progress and demonstrable deliverables.
	• NIST and NASA should use their research experience to help to mentor industry in best practices for computational materials.
	• Support development of non-standard characterization and testing methods.
	• Create an industry group to develop requirements for an ICME framework (including V&V, UQ, etc.).
	• Develop a broader joint roadmap for technology developers (including educators), end users, and regulators.
	• Provide increased emphasis on workforce training and development.
	• Champion standards development.
	• Develop improved capabilities for:
	  • Quantitative in-situ micro-structure characterization and evolution.
	  • Probabilistic methods and Uncertainty Quantification.
	  • Developed improved capabilities for NDE of thick additive parts (high-z, complex configurations)
	  • Micro-structure sensitive defect-mediated durability, damage tolerance, fatigue.
	  • Accelerated high-cycle fatigue tests and models.
	  • Simulation of micro-structurally small crack initiation and propagation.

10 years: • Make the connection between the set of process parameters and the local state of the material for a wide range of materials and conditions. • Develop best practice guides for achieving a specific material state by adjusting the qualified build parameters. *20 years:* • Develop specifications that will lead to build characteristics that are consistent between multiple machines and multiple machine vendors. Provide statistically valid data to demonstrate this consistency. Note that this is a 20-year goal largely because rapid changes in the state-of-the-art makes this a moving target.	

3. Summary and Next Steps

This report documents the goals, organization, and outcomes of a TIM on Computational Materials Approaches for Qualification by Analysis held at NASA Langley Research Center on January 15-16, 2020. The TIM was co-organized by NASA, NIST and the FAA. Approximately 60 SMEs representing 8 aerospace manufacturers, 7 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 regulatory organizations and aerospace manufacturers with participation being roughly evenly divided among the processing and performance tracks. During this TIM, the future needs of the aerospace manufacturers, coupled with the corresponding regulatory considerations, motivated the overall discussion and framed the input given by the government laboratories and universities.

As discussed in this report, the key objectives of the TIM were to understand existing gaps in model-based, 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. Several representative computational materials capabilities that were identified as being enabling and that NASA, NIST and other government agencies should consider supporting include:

Track 1 - Process-Microstructure
- Development, integration and implementation of physics-based and data-driven approaches.
- Development of a framework for defining and implementing model maturity levels, with specifications for V&V at each step.
- Methods for simulation of the relationships between process parameters/compositions and microstructures for a range of build parameters and machines.

Track 2 – Microstructure-Performance
- Integration of computational-based design for inspectability within the design process.

- Increased emphasis on methods for probabilistic simulation and uncertainty quantification.
- Development of non-standard characterization and testing methods.
- Quantitative in-situ micro-structure characterization.
- Accelerated high-cycle fatigue tests and simulations.
- Micro-structurally small fatigue crack initiation and propagation including effect of defects.

Following the breakout sessions, attendees participated in a closing discussion that addressed the following near-term issues:

- Means by which the outcomes of this exercise can be made actionable.
- Development of closer working relationships with NASA, NIST and FAA.
- Prioritization of future activities and pre-competitive collaborations with OEMs.

The participants widely agreed that, while the discussions were valuable, extensive follow up work is necessary to coordinate a National effort on computational materials for Q&C. Several industrial representatives suggested that a small steering group should be assembled to provide input and guidance to the OEMs and regulatory agencies on how computational materials methods should be matured so that they can be effectively used in the context of a Q&C framework aimed at decreasing the time and cost of qualifying and certifying materials and components produced using process-intensive manufacturing methods. The steering group should not only consider “a phased approach at 5, 10, 20 years” as discussed during the TIM, but also seek earlier intermediate outcomes that can be achieved within the next 2-3 years. The resulting Computational Materials for Q&C (CM4QC) Steering Group was formed in the Fall of 2020 and has begun to pursue many of the goals discussed in this document.

Appendix A: Program Agenda

NASA / NIST / FAA TIM on Computational Materials Approaches for Qualification by Analysis

January 15-16, 2020
NASA Langley Research Center
Integrated Engineering Services Building (2102) Room 263
Hampton, VA 23681

Organizing Committee

Ed Glaessgen, NASA
Lyle Levine, Alkan Donmez, Paul Witherell, NIST
Michael Gorelik, FAA

Objectives of the TIM

The key objectives of this TIM are to explore existing gaps in model-based (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 qualification and certification (Q&C), with an emphasis on process-intensive metallic materials technologies. The output of this TIM will be used, in part, to further refine current and future programs in order to support future Q&C efforts for advanced metallic material systems in Aerospace applications.

Agenda

January 15, 2020

Opening

7:45-8:15	Arrival, Registration and Agenda Overview	
8:15-8:30	Welcome and Opening Remarks	Jonathan Ransom Deputy Director for Structures and Materials, NASA Langley & Mary DiJoseph Aeronautics Research Director, NASA Langley

SOA of Computational Materials and Predictive Capabilities

8:30-9:00	SOA of Computational Materials	Greg Olsen QuesTek Innovations
9:00-9:30	Center for Materials in Extreme Environments	Jim Belak Senior Scientist, LLNL
9:30-10:00	Break	
10:00-10:30	Example of Industry Activities Toward Development of Predictive Durability Assessment	Michael Gorelik Chief Scientist for Fatigue and Damage Tolerance, FAA

Series of 20-Minute Presentations from Members of the Aerospace Industry
Speakers have been asked to:

- *Address key questions* posed by the organizers for up to 20 minutes*
- *Present other topics of interest to their corporations for any remaining time*

10:30-10:50	Lockheed Martin Perspectives	Rick Barto
10:50-11:10	Boeing Perspectives	Nate Ashmore
11:10-11:30	P&W Perspectives	Vasisht Venkatesh
11:30-12:30	Lunch in the Afterburner, adjacent to main dining room of the cafeteria	
12:30-12:50	Bell Perspectives	Jerry Nanni
12:50-1:10	Other thoughts from the OEMs	OEMs

Regulatory Considerations and Standards

1:10-1:40	NASA AM Standard	Doug Wells Deputy Technical Fellow NASA MSFC
1:40-2:10	Regulatory Considerations for Modeling and Simulation	Michael Gorelik Chief Scientist for Fatigue and Damage Tolerance, FAA
2:10-2:30	Observations/Thoughts from Participants	All
2:30-3:00	Break	

Input from the OEMs and Aerospace Community

3:00-3:30	Instructions, break and divide into tracks	

Track 1- Process to Microstructure
Track 2 – Microstructure to Performance

3:30-5:00 Address Group 1 questions

5:00 Adjourn Day 1

January 16, 2020

8:00-8:30 Arrive and convene Day 2

8:30-10:00 Address Group 2 questions

10:00-10:30 Break

10:30-12:00 Address Group 3 questions

Closing Discussions

12:00-12:30 Lunch “to go” from cafeteria

12:30-1:30 Working Lunch - Report Out (30 minutes summary/track)

1:30-2:00 Closing discussion
- How can we make outcomes of this exercise actionable
- Closer working relationships with NASA, NIST and FAA
- Future activities and pre-competitive collaborations with OEMs

2:00-2:15 Closing Comments for Day 2
Final opportunity for comments from the participants

2:15 Adjourn Meeting

Optional

2:30-5:00 Informal presentations, side discussions, laboratory tours
For those who are interested and available, we can arrange any interactions with NASA, NIST or FAA that might be of interest. Just let the organizers know.

Appendix B: List of Participating Organizations

Air Force Research Laboratory
Bell Textron
Boeing Research and Technology
Carnegie Mellon University
Collins Aerospace
Federal Aviation Administration
General Electric
Joby Aviation
Lawrence Livermore National Laboratory
Lockheed Martin
National Aeronautics and Space Administration
National Institute of Standards and Technology
Office of Naval Research
Pratt and Whitney
QuesTek
Sandia National Laboratory
United Technologies Corporation (now known as Raytheon Technologies Corporation)
University of Texas – San Antonio

Appendix C1: Complete List of Questions and Responses for Track 1 – Process to Microstructure

Group 1 questions - Qualification Gaps, SOA and Challenges
Facilitator: Eddie Schwalbach, AFRL
Notes: Andy Ramlatchan, Wes Tayon, Josh Fody, NASA Langley

Question 1: What gaps cannot be addressed using traditional qualification methods or processes?

- Challenges with local variation and spatial dependence; cannot characterize full volume of parts.
- Continuous Cooling Transformation and Time Temperature Transformation curves are not detailed enough to obtain properties; missing important properties such as dislocation density.
- Nucleation rates and epitaxy to nucleation are all empirical.
- If one wants to understand evolution, one must have thermo-kinetic modeling for which cooling rates are needed. There is a need to couple mechanistic and thermo-kinetic models.
- Coherency and strain fields in precipitate formation.
- How to obtain appropriate microstructure into test coupons? Can models be used to assist this process?
- Is tensile test data proprietary? Can we convince OEMs to share test data which may not be proprietary?
- Cost and time considerations to develop large statistical databases are a challenge, specifically, when different structure and properties throughout the volume of a part are considered.
- There is currently no way to obtain the same microstructure at different locations within a complex geometry.
- The all-variables-locked approach cannot handle variable processes.
- The process database is controlled by microstructure rather than allowables. What is the “minimum viable dataset” for reproducibility? What needs to be included? Can computational materials approaches help to address these issues?
- Limited microstructure considerations are explicitly included in the qualification process; how do microstructure models play a role?
- Lack of transparency in understanding processing details is a concern. Commercial machines are operated as black boxes.
- Data driven vs. physics-based models; robustness is a concern with data driven approaches alone. What is the role of hybrid approaches?
- The effect of recycled powder usage has not been well-captured. This issue should be investigated.
- Understanding and accounting for machine-to-machine variability is needed.
- How can data be obtained more generally considering intellectual property considerations in light of the black-box nature of machines.

Question 2: What is the current SOA for computational materials, including examples of success stories?

- HRL Laboratories' use of informatics/CALPHAD to select appropriate alloying elements for printable 7000 series Aluminum.
- Maturity/utility of CALPHAD tools with the caveat that databases are not necessarily comprehensive and may not be continuously updated.
- Determination of which microstructural features are most impactful to properties (for new alloys, and/or new processes) and therefore should be measured/predicted. For old alloy/new process situation, are these necessarily the same as they would be for conventional materials?
- Both the as-built and final microstructure are relevant. The as-built microstructure becomes the initial condition for design of the post processing steps.
- Prediction of micro-segregation is needed. There have been successes, but best approaches to date have used data driven approach/extrapolation.
- Phase-field has been useful for understanding behaviors generally but is not currently practicable on real (many component) alloys.
- Macro-scale or part-scale residual strain and distortion modeling for L-PBF is commercially available and is becoming relatively mature. There are questions about quantitative accuracy although the tools have demonstrated qualitative value. A gap is coupling to microscale strains, dislocation densities and local microstructure.
- Power-Velocity (P-V) maps are used by industry to avoid several defect mechanisms; however, the approach requires additional development, including work to develop P-V maps for fatigue and to consider complex part geometries.
- Existing process modeling tools like DEFORM and ProCast used for "conventional" processes are commercial and mature; varied degree of coupling/capability at the microstructural level, but they are used to reduce time to first article.
- High fidelity L-PBF process model from Lawrence Livermore National Laboratory to identify importance of various phenomena is expensive and not tractable at the part scale so it motivates careful multi-scaling.
- Computational tools are still valuable even if they do not enable complete certification by analysis; models to facilitate/compliment/guide empirical efforts, identify relevant physical phenomenon, improve direct testing and eliminate some pathologies early.
- Model uncertainty still needs to be addressed.

Question 3: What are the main qualification challenges that may be addressed by computational materials-enabled capabilities?

- Opportunity for data driven approaches to build a link between in-situ monitoring data and location specific microstructure.
- Prioritization of the phenomena that create the most uncertainties.
- Missing critical thermo-physical data for materials models. Viscosity of liquid and surface tension as function of temperature.
- Use of computational materials to evaluate alloys/perform alloy design for the AM process window and increase robustness of variable processes.

- High fidelity models are valuable to understand process and generate a database but currently do not significantly advance Q&C because they are too scale limited and time intensive.
- Data driven approaches for in-situ process monitoring are likely to assist with developing stable processes. The inclusion of a data driven approach to incorporate microstructure and final properties ensures greater robustness in process certification.
- Computational tools are needed to understand machine to machine variability, (serial number to serial number, as well as model to model, transfer knowledge gained from one system to another). One way to avoid calibrating machine parameters is to specify a final microstructure regardless of what individual process parameters are input for a given machine.
- Process qualification: address/improve predictability of the 'tweak' scenario, i.e., does a seemingly 'minor' change really require re-work or will the process still lie within the acceptable window? Having alloys that are designed to be robust over range of process parameters is important.
- Computational tools to perform sensitivity analysis, such as determining parameters that would be the most valuable to better control, monitor, or measure?
- Computational data package to support transition and coupling across multiple disciplines (materials, structures, designer).

Group 2 questions - Leveraging of Related Capabilities and Organizations
Facilitator: Tony Rollett, Carnegie Mellon University
Notes: Andy Ramlatchan, Wes Tayon, Josh Fody, NASA Langley

Question 4: How can the current or near-term use of computational materials in non-qualification frameworks be leveraged to mature the capabilities for qualification; developing a pathway for leveraging?

- How do we leverage capabilities across organizations and what do those look like for modeling? From the OEM perspective, it would be helpful to understand how to use computational tools to support proposals for, e.g., materials substitution to regulatory boards (FAA, Air Force, NASA, Navy etc.).
  - What models are accepted by material substitution board? Are there examples of success stories? Can we drive a material through the acceptance process largely through computational means? Establishing confidence in models will help significantly.
  - Unlike the structural mechanics community, many materials SME's lack familiarity with computational tools. What meta-data is needed to help build that confidence level with regulatory bodies?
  - Are there opportunities to develop MMPDS tools supported and informed by computational tools?
  - Open source tools can be used once regulation boards have accepted them. Tools have to be approved by regulatory agencies.
- Use of tools to predict variation (e.g., P-V maps); many process-to-structure relationships are unvalidated – many models are as yet unvalidated.
  - Variation in part performance is currently an impediment and requires additional characterization and testing. What is the uncertainty band between "bad" (LOF or

    keyhole porosity prone) and good build parameters in P-V space? Many process models are unvalidated. Having databases would help with validation.
  - Some level of acceptance for use of P-V in powder beds. What simulation tools could help us "draw the lines" in P-V maps, and what can help to validate those lines. We can simulate those lines, but will industry accept particular lines (for each individual machine). Fundamental agreement for P-V maps and variables to be considered. Currently, P-V adjusts elementary variables; however, there are many additional variables including hatch spacing, pre-heat, scan pattern etc.
  - Using a P-V map (e.g., in a qualification document) can create a conflict in the future. Need for a P-V map for qualification to be expandable over time; needs to be updatable at some time intervals.
  - Importance of using simulations to make connections between in-situ monitoring and the defect state for generating P-V maps.
  - P-V maps can lead into (or be used as the basis for) *Best Practice Guides*. Ways of articulating knowledge to develop ways or suggestions for how people approach these problems. Best practice guides can also make a connection to regulatory agencies.
- Matching parameters of importance from computational materials to available measurement capabilities and match the computational parameters that are highly sensitive to the measurement capabilities (e.g., melt pool length and cooling rate of individual tracks, surface tension).
  - Melt pool lengths are important. Solidification boundary is estimated rather than being directly measured. Need to know an estimate from the computational model and compare the experimental measurements.
  - Modelers need better (experimental and/or simulated) estimates of fundamental parameters including surface tension and viscosity of melted material as a function of temperature.
- Even though the business case for using AM clearly exists, how does a computational capability help OEMs to both close the business case for AM and expand its scope.
  - Is there a business case for AM and process intensive materials processing in general (i.e., is it still of interest to use AM in the future or only as a prototyping tool?).
  - Any computational methods that can help to address overarching issues (e.g., machine to machine variability) should be considered.
  - Although there is a strong business case for AM, a challenge is that the methodologies used today to develop AM materials only work in small niche cases. To expand AM use, need to develop further; computation can help.
  - Need to have enough parts and part families to justify use of AM. Qualification for each machine is needed. Computational materials methodologies can help to mitigate existing machine variability. OEMs need help with tool development that will allow them to expand beyond existing products. Collective database to leverage and share data would help to expand use, reduce cost and expand business case.
- An aspirational goal would be to set a limit on surface roughness and use computation to suggest process parameters to stay below that target.

- Models and simulation tools are only as good as the input data. Additionally, simulation of processing can be computationally expensive, so consideration of process variation may not be practical. Additionally, failure modes associated with processing are as important as variation (e.g., disruption of spreading process). OEMs would welcome studies of how well various simulation tools work for a given application.
- How mature does a model have to be used for qualification? Is there an existing capability that is generally agreed to be sufficient? Is there an existing capability that can be augmented? An example for casting is ProCast and how it is being used for qualification of castings.
  - OEMs use both commercially available and internally developed tools. Are the assumptions used in those simulations valid? Has too much of the operative physics been removed for the output to be valid. How well are those models, including derivative reduced order models, validated?
- Machine learning can be used to increase computational output for validation. There may be an opportunity for academics to take multiscale approach in collaboration with OEMs and to see if approaches are experimentally feasible.
  - Need to validate model assumptions first before validating model results. Perhaps there is a role for machine learning in this respect. There may be an opportunity for national labs and government agencies to collaborate with OEM. Start by using all physics possible and systematically decrease fidelity to develop reduced order models that are within an acceptable realm of accuracy.
  - Are there fundamental physical processes that are missing in existing models? Can OEMs share data to enable machine learning approaches? Although this approach might not be possible for production parts, could exemplar parts be considered. Would such an approach still be valuable even though production parts may be significantly different; hence, the exemplar parts may not be representative. Are there exemplar parts that exhibit a variety of desired microstructures?
  - Although the issue will be addressed in the third session, a gap is the lack of a methodology for defining the trustworthiness of models generated via data-driven approaches.
- Models cannot be validated without knowing the final result. How can accurate models be developed without being able to measure properties of interest?
- X-ray Computed Tomography (CT) scans are still not robust enough to be a tool for qualification of AM parts. Can other industries offer experience and capabilities that help mature CT for qualification of AM parts?
- Computational materials approaches are needed to support alloy development and find lower cost alloys for AM. How can we exploit models to predict microstructures and produce the desired microstructures in a given part?
- What is our ability to predict microstructure throughout an AM build? What is the computational cost? Need a lower cost qualification tool. Are there simulation capabilities to support change management as a machine changes over time. A collaborative database may help.

  - Need low-cost capabilities to qualify processing across machines – are there models that can predict machine variability over time and inform the inspection schedule. Are there tools to rapidly qualify and certify new machines?
- X-ray CT is the gold standard for NDE; however, some parts cannot be examined via X-ray CT. There are ways to reduce the data, including dimensionality reduction, compression, etc. Yet, X-ray CT can still result in Terabytes of data from a build and becomes a big data problem both for in-situ data and post-process data.
- In the short term, computational materials may be able to accelerate the production of new alloys. Is there some fundamental physics that we are missing in these models that we as a community can identify and address in the short-term? This could be a good topic for a follow-on technical workshop. Also, is there a part of the process where everyone would be comfortable sharing data within the community.
- Is there a set of generic geometries that exhibit a variety of location-specific microstructures? Are there complex geometries that capture a variety of processing parameters?
- How many parameter combinations will produce a desired microstructure, i.e., is there a many-to-one mapping for process settings to microstructure? Is there a way to produce or establish a standard microstructure for a given material?
- Is there set of documents that NASA or NIST can generate toward a computational materials-informed specification for AM?
- Three criteria must be addressed to support model competency: model uncertainty, process uncertainty, measurement uncertainty. Do we have a proper uncertainty budget for each of those criteria? Measurement capabilities that bridge gaps can reduce uncertainties.
- Model uncertainty can be a measurement for model maturity.
  - In industry, there are established TRL / MRL for processes and technologies. A similar scale is needed to assess model maturity levels. Is there a framework to establish something similar for models and rank their level of validation?
- Need input from OEMs for developing standards and benchmarking activities. There are computational benchmarks as well (e.g., Exascale simulation on supercomputers).

Question 5: Are there any competition insensitive ways to share information (pre-competitive)? Is there a pathway to leverage internal company capabilities for use by the larger community?

- There is some opportunity related to raw test data. The greatest sensitivity for companies is in the use of data for development of design allowables.
- There is also the possibility of sharing data from the Metals Affordability Initiative; however, the challenge is to obtain a release from all the participating companies.

Question 6: Is there a role that industry working groups/standards organizations could play in this process? Where do the standards opportunities lie?

- A suggestion was made to set up a Steering Group (industry), that could identify high priority issues. Note: that group has since been established and is led by NASA and the FAA.

- A significant opportunity might be to develop guidance for addressing the many regulatory bodies (e.g., DoD Airworthiness, JSSG-2006, MILT-STD -1530D, AWB-1015, FAA) to which companies must submit regulation-related packages. Such interactions (and packages) do not typically include computational materials-related information.
- An interesting point was made that the geometry-based approach to allowables is unlikely to work because of the complexities introduced by the AM process.
- The use of Process Equivalent Test Specimens (PETS) applies to all processes and technologies, not just AM, so this could represent an opportunity for the Steering Group (and equivalent bodies) to consider.

Group 3 questions - Capability Development

Facilitator: Lyle Levine, NIST

Notes: Andy Ramlatchan, Wes Tayon, Josh Fody, NASA Langley

Question 7: What is the role of V&V and Data Science in the maturation of computational materials capabilities?

V&V

- Availability of reliable measurement data is limited; there is often not enough of this high-quality data to validate the needed models and simulation tools. Greater access to such data is necessary for V&V aimed at maturing computational materials capabilities. Improved coordination and communication between measurement teams (NIST, NASA, AM-Bench, etc.) and OEM simulation teams would allow measurement priorities to better reflect OEM needs.
- The prioritization of measurement needs must target factors that have a strong effect on the manufacturing processes. Sensitivity analyses and design of experiment approaches may prove useful in identifying such measurement targets.
- The quantitative values and functions of thermophysical parameters used as inputs into the models has a substantial impact on V&V. A good example is the temperature dependence of the surface tension of metal alloy melt pools; this drives the Marangoni flow that affects the melt pool geometry during laser powder bed fusion.
- Procedures and standards for calibrating both the build parameters and the in-situ monitoring systems is critical for making build systems interchangeable. Part of this effort would be to determine how sensitive the build process is to each input parameter and how accurately these parameters must be maintained to provide a reliable and interoperative build system.
- A limitation of current in-situ monitoring systems is the lack of clarity regarding precisely what is being measured and how these measurements relate to the AM build's microstructure (including defects). Bridging this gap between the measurements and the microstructure would have a major impact on build quality, throughput, and interoperability of the build machines. Another related issue is the determination of which in-situ monitoring systems are best for a given purpose.
- Another important requirement for measurement data used for V&V is the need for metadata. Perhaps the most important issues related to this requirement as related to commercial

systems are the determination of the information that constitutes the most important metadata, availability of raw measurement and monitoring data and accurate descriptions of the metadata.

Data science

- When possible, data types within a given study should be acquired and stored consistently (e.g., fields of view, contrast, data formats).
- Machine learning may prove to be extremely useful in the future; however, the quality and inter-applicability (e.g., between machines) of the training data are key enablers for its application.
- Storage, transportation, and analysis of large data sets are recognized problems that must be addressed, but attention also needs to be made to the wide variety of data sets needed to validate models. Care must be taken to ensure a proper intersection between measurement outputs and modeling requirements.

Question 8: What is the appropriate balance between modeling and testing for a fully mature computational materials framework (end state vision) to achieve the desired state for next-generation (computational materials-enabled) qualification?

- The appropriate balance between modeling and testing is informed by community input, communication and prioritization. Lessons learned from other domains (e.g., aerosciences including computational fluid dynamics) may provide guidance regarding the extent to which simulation can replace testing. The appropriate balance is also largely determined by those organizations that are responsible for certification.
- Issues include:
  - Development of formal procedures and metrics for testing simulation predictions would provide confidence in the simulation outputs. Currently, it is often not clear what the critical tests are for validating the simulation outputs. Although no formal method for their determination exists, there are internal procedures that specific OEMs and academics use.
  - A barrier that limits the development of formal procedures and metrics is that disconnects often exist between what can be measured and what is perceived to be required. An example is stress, which is not a measurable quantity. In this example, a connection could be made to the actual measurands such as lattice parameters (if using diffraction to elucidate the local stress state).
  - Another barrier is that quantitative simulation often requires accurate and precise inputs, but there is typically little understanding of how accurate and precise the inputs need to be.
  - Machine learning (ML) could play a major role in filling some of the knowledge gaps and would be significantly faster than complex computational techniques. However, major barriers exist in making ML both reliable and extensible between different build machines and situations.
- A related, and important, enabler for achieving a good balance between modeling and testing is related to the introduction of alloys that are specifically designed for AM. For example,

alloys could be designed that are less sensitive to AM process variations. This expanded process window would improve performance reproducibility and decrease machine-to-machine variability, thereby decreasing the need for extensive testing.

Question 9: What capabilities should NASA & NIST champion to enable next-generation qualification of process intensive metallic materials (e.g., AM). What is the timeline and phased approach at 5, 10, 20 years?

All years:

- NIST (AM-Bench) and NASA can provide robust data for simulation V&V. Another source is DoD (AFRL Challenge Series).
- Consider both physics-based approaches and data driven approaches.
- Develop an understanding of the inherent sources of variability – not just with machines, but in the AM process itself and in the feed stock.
- Work with partner organizations to develop improved mechanisms and guidance for acquiring and sharing both data and metadata.

5 years:

- Provide guidance for measurements and calibrations that can be used to validate basic sets of process parameters to support qualification of both process parameters and machines. Example parameters for laser powder bed fusion include laser power, scan velocity, laser power distribution function and hatch spacing.
- Make the connection between the complete set of process parameters and the local state of the material for a narrow set of materials and conditions. This goes beyond existing P-V maps that only address two process parameters.
- Develop a framework for defining and implementing model maturity levels, with specifications for V&V at each step.
- Although a given feedstock chemistry typically falls within formal alloy specifications, these specs are often broad enough to introduce substantial variation in the part performance. Work with standards organizations such as ASTM to address this problem of material specifications for AM feedstocks.

10 years:

- Make the connection between the set of process parameters and the local state of the material for a wide range of materials and conditions.
- Develop best practice guides for achieving a specific material state by adjusting the qualified build parameters.

20 years:

- Develop specifications that will lead to build characteristics that are consistent between multiple machines, multiple machine models and multiple machine vendors. Provide statistically valid data to demonstrate this consistency. Note that this is a 20-year goal largely because of the rapid changes in the state-of-the-art.

Appendix C2: Complete List of Questions and Responses for Track 2 – Microstructure to Performance

Group 1 questions - Qualification Gaps, SOA and Challenges
Facilitator: Michael Gorelik, FAA
Notes: Sai Yeratapally, David Wagner, Andy Newman, NASA Langley

Question 1: What gaps cannot be addressed using traditional qualification methods or processes?

- Capturing variability and distribution of rogue anomalies.
- Lack of the standard micro-mechanical properties needed to characterize a microstructure.
- Lack of standardized models and understanding of underlying physics needed to transfer properties from micro to macro scales.
    - Standardized models exist for some properties, but not all (e.g., fatigue). Probabilistic fatigue analysis shows promise here.
    - A representative volume for AM materials is not well-defined?
    - The path for leveraging traditional approaches for Q&C to AM is unclear.
- Unknown types and characteristics of defects stemming from powder properties.
- Determining the effects of powder recycling.
- Long-term performance evolution under cyclic loading and service environments (e.g., aging, environmental degradation).
- Determination of the critical defect size.
- Complex and challenging (e.g., thin wall) internal features are made possible by AM but likely have location-specific microstructure and may not be inspectable.
- Effect of cleaning and post-processing, especially with respect to repair of defective parts.
- Interaction of microstructure and porosity and their combined effect on material performance. At what size distribution of porosity does micro-structure dominate performance?
- Characterization of micro-structurally short fatigue crack growth in materials with defects.
- Determination of the effects of non-equilibrium micro-structure, primarily, in as-built conditions.
- Determination of the effects of residual stresses on performance
- Understanding of fatigue crack initiation and microstructurally small crack propagation in AM materials.

Question 2: What is the current SOA for computational materials, including examples of success stories?

- SOA for electronics (semiconductors) is mature, from ab initio to atomic to continuum scales and can be used as a benchmark.

- State of Practice lags State of the Art. Most computational materials capabilities have not matured beyond use in the laboratory environment.
- Computational non-destructive evaluation and big data analytics are being adopted for research, with interest by OEMs.
- Some aspects of Computational Materials are as much of an art as they are a science.
- computational materials simulations should be based on informed, rather than simply convenient, approximations.
- The trend is toward forward-calculating (predicting) observable experimental results using results from sensitivity studies, including, understanding which inputs have the most influence on performance.
- Calibrated continuum material models are used routinely to predict performance.
- A list of success stories includes:
  - Success Story 1: Three-dimensional microstructure observations (e.g., synchrotron-based high energy diffraction microscopy) in research
  - Success Story 2: DREAM.3D for generating micro-structure models.
  - Success Story 3: DREAM.3D and crystal plasticity for NASA commercial crew program.
  - Success Story 4: Use of Probabilistic Damage Tolerance for safety-critical engine component certification.
  - Success Story 5: New probabilistic high-cycle fatigue models that account for some microstructural features.
  - Success Story 6: Development of methods based on machine learning and reduced-order models to replace expensive high-fidelity computational methods.
  - Success Story 7: Microstructure to location-specific bulk properties has been demonstrated in practice for some materials.

Question 3: What are the main qualification challenges that may be addressed by computational materials-enabled capabilities?

- Cost, time and minimization of the number of required tests.
- Simulation beyond experimental limits. Validation is a concern.
- Uncertainty quantification and uncertainty management.
- Quantifying the effects of defects.
- Development of a Digital Twin, including quantitative condition-based maintenance.
- Determination of a critical initial flaw size.
- Determination of location-specific properties.
- Parametric studies to understand variables that are difficult to control experimentally.
- Use of computational materials simulations to optimize experiments and develop test matrices.
- Development of transfer functions from test coupons to components.
- Application of data analysis to simulation results before applying to experimental results.
- More efficient material and hardware acceptance.
- More rapid Materials Review Board disposition.
- Changing the paradigm from Point Design to Part Family qualification.
- Transferring qualification from machine to machine.
- Full material and hardware design concurrency.

Group 2 questions - Leveraging of Related Capabilities and Organizations
Facilitator: Harry Millwater, UTSA
Notes: Sai Yeratapally, David Wagner, Andy Newman, NASA Langley

Question 4: How can the current or near-term use of computational materials in non-qualification frameworks be leveraged to mature the capabilities for qualification; developing a pathway for leveraging?

- Leverage NIST AM-Bench, ASTM AM COE as known/trusted/validated standards for comparison.
- Communication needed between regulatory and industry organizations. Develop roadmaps to highlight future needs for toolsets, including involvement of standards development organizations such as ASTM and NIST.
- Tool maturation to bridge entire process-to-performance space is needed. Overall, the volume of data/information is insufficient for qualification; however, some success stories exist (e.g., landing-gear steels).
- Use computational models to interpret in-situ monitoring and/or other intermediate steps in the ICME process, including:
  - Build confidence progressively/gradually; coupons to parts; point design to part families; develop intermediate technology that will be required for final certification independent of part criticality.
  - Build success stories by partnering with non-aerospace industries (e.g., the maritime industry). Work their "easy" problems to build confidence. Similarly, low-criticality aircraft applications can fill this role.
  - Provide assistance with models, not just "anchoring" models, by providing insight vs. specific and explicit predictions.
  - Develop validation framework pedigree, including credibility with certification authorities. Need to show models are as credible as test data/results.
- Need to invert the current process to certify general processes for classes of materials rather than specific parts/processes/materials.

Question 5: Are there any competition insensitive ways to share information (pre-competitive)? Is there a pathway to leverage internal company capabilities for use by the larger community?

- Not just data, but knowledge and information, should be shared. Data is important, but the combination of data and models may provide greater insight and knowledge.
- Often, existing government-owned data is not shared (even between government agencies). This practice is not helpful and should be changed.
- Standard form of data exchanges is not straightforward (e.g., materials engineers want different data than mechanical engineers).
- Advancing some aspects of the state-of-the-art requires sharing of information rooted in competitive results; therefore, efforts are required to turn competitive data into a non-competitive format.

- Developing trust with data/models generated by others is required (i.e., establishing data/model pedigree).
- A list of success stories includes:
  - NASA Advanced Composites Program NDE handbook developed a sharable NDE standards/data library supported by round-robin testing by different entities and different NDE methods. It may be a model for management of sharable physical and electronic libraries.
  - FAA-sponsored Turbine Rotor Material Design, RISC working group where data was "pooled."
  - Metals Affordability Initiative (MAI).

Question 6: Is there a role that industry working groups/standards organizations could play in this process? Where do the standards opportunities lie?

- Consortia of industry/federal groups to help standardization organizations and serve as a steering group to provide vision.
- Communication is needed between regulators, industry and standards development organizations (e.g., ASTM, NIST) to support development of roadmaps that include future needs for toolsets.
- FAA is moving towards performance-based regulations rather than prescriptive regulations, i.e., moving away from defining means of compliance. In the future, public standards will define means of compliance.
- Calibration of codes and methods may be addressed by government organizations, e.g., NIST.
- Need standards of application programming interface (API) for code access and standardization of data between codes, e.g., schema. A success story is the NDI sharable models working group. Such standardization helps to support transferability.
- Establishment of benchmarks are needed to provide standard sets of data.
- Standards need to be expanded to support AM (e.g., allowable O, N content in alloys).

Group 3 questions - Capability Development
Facilitator: Corbett Battaile, Sandia
Notes: Sai Yeratapally, David Wagner, Andy Newman, NASA Langley

Question 7: What is the role of V&V and Data Science in the maturation of computational materials capabilities?

- Development of capabilities for performance-limiting feature recognition in in-situ process monitoring.
- Standardized V&V and UQ supporting uncertainty management protocols.
- Capturing sensor-based data process parameters for model validation.
- Defining guidelines for characterizing model maturity and validation level (i.e., analogous to TRL).

- Increasing ability to couple NDE data with computational materials models for effects of defects
- Data science and big data management are essential for timely validation as models become larger and more complex. Examples include:
  - Extracting usable information from terabytes of source data to identify what information is needed.
  - Support of standardized raw data formats and data storage protocols.
  - OEMs have noted a lack of protocol/infrastructure/conduits for moving/transferring big data to its end uses.
- Development of validation approaches to provide coverage over multi-dimensional parameter spaces.
- Calibration of non-linear material model parameters under UQ and V&V.
- Consider NAFEMS (nafems.org) as a model for finite element models and data best practices.
- V&V is a prerequisite for the use of computational materials in the Q&C framework.
- Need an agreed-upon framework for V&V as a function of application and domain.
- Model developers should be aware of V&V requirements from the initial states of model development for the support of Q&C. Model developers should also have incentives to adhere to these requirements.
- Model developers need a clear plan for generation of user data throughout the process from the initial stages onward in four specific categories, including model development, model calibration, verification and validation.
- One concern is that the scope of V&V is not always well-defined. As an example, codes can be declared as being “validated” without the scope of their domain of validity being described precisely enough for proper use.
- Clearly delineating computational model V&V (and related implementations) from software V&V. If the validation case is accessible, it can be used to validate physics-based models.
- Automated V&V testing of code, supporting software development best practices.
- Industry-accepted data provenance protocols.
- Industry-accepted common data models and API standards.
- Shifting to a paradigm that leverages microstructure constitutive models instead of tables of coefficients to Q&C activities/component properties.

Question 8: What is the appropriate balance between modeling and testing for a fully mature computational materials framework (end state vision) to achieve the desired state for next-generation (computational materials-enabled) qualification?

- Role inversion such that experiments are driven by model validation and calibration needs.
- Balance is dependent on intent (e.g., design) and the acceptable level of risk based on known uncertainties and criticality of a component and on maturity and availability of NDE.
- The appropriate balance will evolve as models mature.
- Development of the risk tolerance level should inform development of the framework. Tighter tolerances will require more testing.
- Validation tests should be targeted to system-critical locations (i.e., system-wide assessment informs component test needs).

- Balance depends on intricacy and difficulty of measuring model inputs in addition to cost and time requirements. For example, measuring micro-structurally small crack growth rates and directions may be prohibitively expensive.
- Continue to advance both testing capabilities and modeling capabilities. This is a two-way relationship since model improvement often requires experimental improvement.
- Modeling can support the context for certification, e.g., materials are certified in the context of a component and the component is certified in the context of a system.
- ASCI may be a model for this balance.
- There is a shift from standardized testing to standardized test design (e.g., to capture coupled loading or actual use loading).
- The optimal balance between running one large, high-fidelity model and many smaller, simpler models, is evolving.
- Models show gaps in experimental methods, thus, informing experimental method development.
- Modeling and data analytics must be combined in an optimal way since data generation can be used to support more than just model development.

Question 9: What capabilities should NASA & NIST champion to enable next-generation qualification of process intensive metallic materials (e.g., AM). What is the timeline and phased approach at 5, 10, 20 years?

- Focus on computational-based design for inspectability integrated into the design process.
- Increased focus on probabilistic and UQ methods.
- Generally, focus on incremental progress and demonstrable deliverables.
- Use research experience to help to mentor industry in best practices for computational materials.
- Development of non-standard characterization and testing methods.
- Create an industry group to develop requirements for a computational materials framework including V&V and UQ.
- Develop a broader joint roadmap for technology developers, educators, end users, and regulators.
- Workforce training and development.
- Computational materials standards development.
- Quantitative in-situ micro-structure characterization and evolution.
- NDE of thick additive parts (e.g., high-z, complex configurations).
- Micro-structure sensitive defect-mediated durability and damage tolerance.
- Accelerated high-cycle fatigue tests and models.
- Simulation and characterization of microstructurally small crack initiation and propagation.

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14. ABSTRACT

This report documents the goals, organization and outcomes of a Technical Interchange Meeting (TIM) on Computational Materials Approaches for Qualification by Analysis, co-organized by NASA, NIST and the FAA. The TIM was held at NASA Langley Research Center on January 15-16, 2020. Approximately 60 subject matter experts (SMEs) representing 8 aerospace manufacturers, 7 government organizations and 2 universities participated. Expertise of the SMEs spanned the Technology Readiness Level (TRL) scale from the low-to-mid TRL focus of government laboratories and universities to the high TRL perspective of the regulatory organizations and aerospace manufacturers. During this TIM, the future needs of the government regulators and manufacturers 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, 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 qualification and certification (Q&C).

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