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USING ADDITIVE MANUFACTURING AS A PATHWAY TO CHANGE THE QUALIFICATION PARADIGM

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Abstract

Additive Manufacturing (AM) offers the opportunity to transform design, manufacturing, and qualification with its unique capabilities. AM is a disruptive technology, allowing the capability to simultaneously create part and material while tightly controlling and monitoring the manufacturing process at the voxel level, with the inherent flexibility and agility in printing layer-by-layer. AM enables the possibility of measuring critical material and part parameters during manufacturing, thus changing the way we collect data, assess performance, and accept or qualify parts. It provides an opportunity to shift from the current iterative design-build-test qualification paradigm using traditional manufacturing processes to design-by-predictivity where requirements are addressed concurrently and rapidly. The new qualification paradigm driven by AM provides the opportunity to predict performance probabilistically, to optimally control the manufacturing process, and to implement accelerated cycles of learning. Exploiting these capabilities to realize a new uncertainty quantification-driven qualification that is rapid, flexible, and practical is the focus of this paper.

Introduction

Additive Manufacturing (AM) is a flexible, agile production pathway ideal for low volume, high value, high consequence, complex parts that are common in high-risk industries such as defense, energy, aerospace, and medical [1,2]. To achieve a paradigm shift in qualification using the promise of AM there are multiple technical challenges that must be addressed. Today, AM processes suffer from challenges with variability in part quality due to build-to-build inconsistencies, inadequate dimensional tolerances, surface roughness, grain size, and defects [3, 4]. These challenges result in costly and time consuming post-build processes (e.g. Hot Isostatic Pressing, machining) to inspect/remediate internal defects (porosity, cracks), alter material properties (strength, ductility), or introduce surface modifications (finish, tolerance). Minimizing these added post-build processes is strongly desirable for financial and qualification needs. Having the ability to predict properties, structure, and performance of AM builds allows for the use of optimization for part performance and the ability to eliminate -- or at least reduce -- post-build processing to specific locations known before the build.

Inherent to the paradigm shift needed to change qualification is the integration of computational and physical models that comprise of a range of material options and incorporate multiple length and time scales. Utilizing these integrated models to produce a validated, predictive capability integrated with real-time and ex-situ diagnostics is the foundation of this approach. The technical challenges to achieve this new paradigm can be divided into five key areas.

1. Novel real-time AM diagnostic tools to quantify and monitor critical AM process variables for materials control and optimization.

2. Innovative and rapid experimental techniques to calibrate and validate models as well as correlate materials performance to in-process diagnostic measurements.
3. Computational models to relate process conditions to microstructure and ultimately to bulk measurable properties.
4. Approaches to characterize, model, and control variability in AM processes.
5. Intelligent data collection from various and diverse sources to develop science-based heuristics.

The need to bridge multiple length and time scales is intrinsic in these technical challenges, which favors an approach that is hierarchical, optimization focused, and science-based. The acquisition of foundational knowledge through novel real-time AM diagnostics [5] and materials assessment techniques ultimately progresses to next-level assemblies and then to full component qualification.

A new qualification approach is motivated by using AM to advance component design [6] and performance. Tight control of the manufacturing process promotes the ability to increase process yields and fosters the ability to predict process performance. Materials can be designed with desired properties for performance while facilitating easier characterization of property measurements for model calibration. Designing model validation experiments for the expected material and component performance provides a direct line to mechanistic model-form development and performance assessments. These validated models elucidate the Process-Structure-Property-Performance (P-S-P-P) connectivity that is difficult or impossible to deduce experimentally. Validated computational models require extensive experimental observations to understand the domain of model agreement or bias and uncertainties in model predictions. Ultimately, as highlighted in Figure 1, using the capabilities of AM integrated with a validated, predictive capability and real-time and ex-situ diagnostic tools facilitates creation of a framework to translate AM Process results to material properties by relating micro Structure to bulk measurable Properties to ultimately predict component Performance.

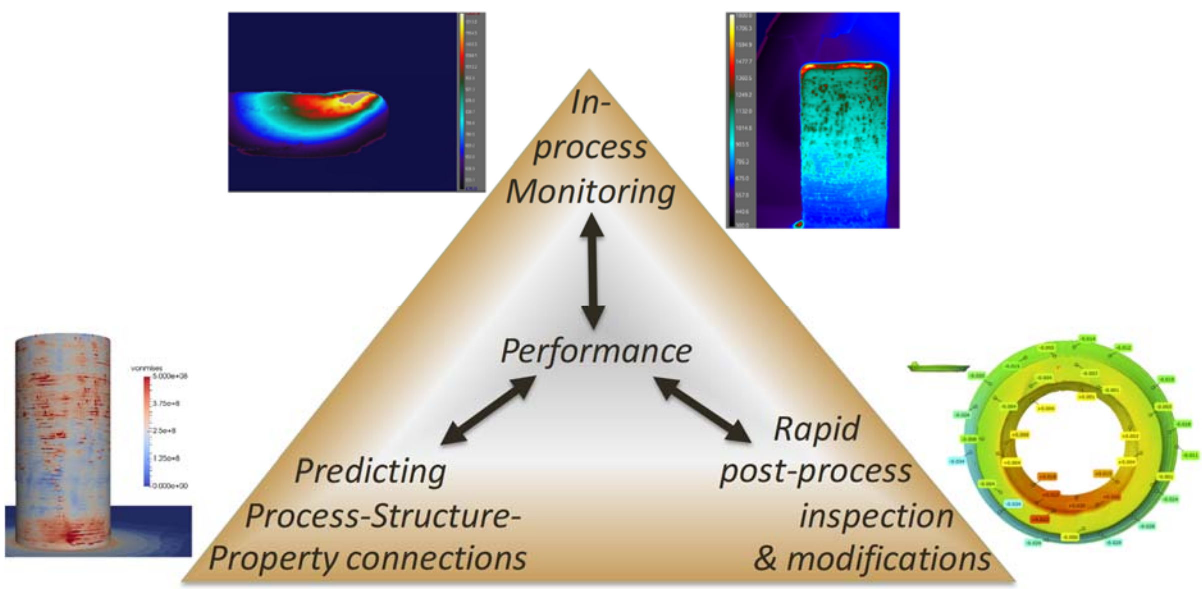

Figure 1: General P-S-P-P approach to development of a New Qualification Paradigm

Another driver in the development of a new qualification paradigm using AM is the ability to decrease the length of the product cycle from design through production. This is especially true for high value, high consequence, complex parts common in high-risk industries where requirements for high reliability often leads to cost inefficiencies, loss of flexibility, and diminished agility in designs. Figure 2 shows a notional construct of how a reduction in cycle time can be achieved. The first reduction, Figure 2b, is in time-to-build using the inherent promise of AM to quickly produce parts and components. A second reduction, Figure 2c, is tied to the ability to predict component performance, greatly reducing the dependence on validation tests of process and performance. These cycle time reductions are partially driven by an expansion of the design phase [7] to allow for a focus on prototype development. Advanced prototyping supports an Accelerated Cycle of Learning [8] approach, where confidence and knowledge is increased with more information available earlier in the product cycle. Overall the improved cycle time is a natural output of using AM to enable probabilistic performance estimation, design optimization, and P-S-P-P connectivity, which are all key requirements to creating new performance regimes for changing design, manufacturing, and qualification.

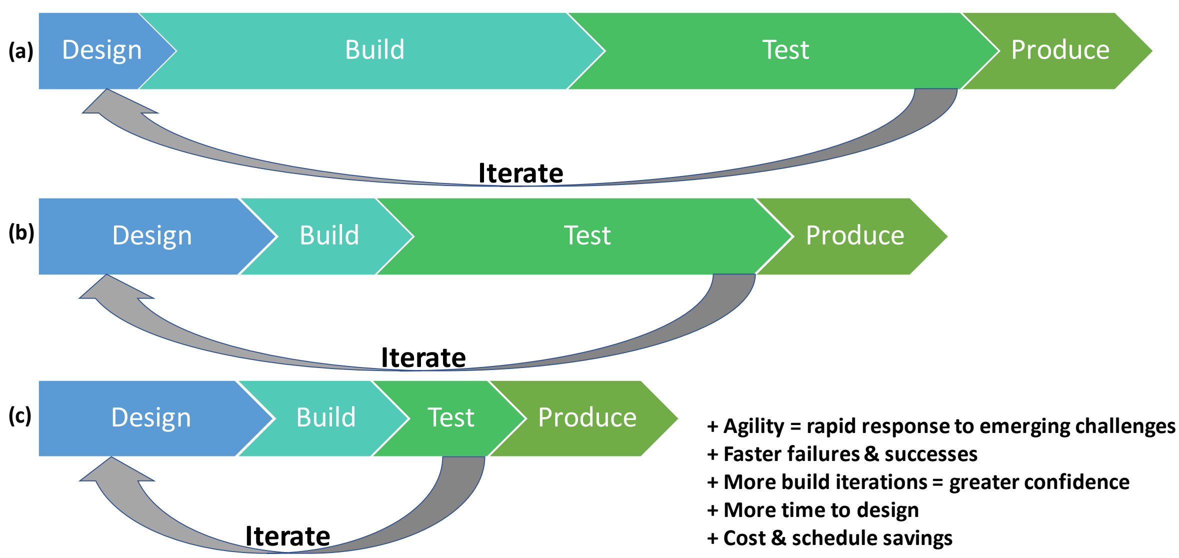

Figure 2: Overview of an improved a product cycle to achieve New Qualification Paradigm, (a) typical product cycle using traditional manufacturing processes, (b) product cycle using AM capabilities, (c) product cycle possible using AM with ability to predict performance

This paper is organized by focusing on the core technical challenges to achieve a new qualification paradigm. Process control and in-situ diagnostic needs and challenges are introduced in **Diagnostics - Process and In-situ**. Process and performance benchmark artifacts are discussed in **Assessing Materials and Process Performance**. The need for capabilities to rapidly characterize materials assessment is covered in **Rapid Characterization**. Modeling and simulation needs to bridge the time and length scales, the need for P-S-P-P connectivity, and the capability to predictive performance is discussed in **P-S-P-P Models**. How data science and optimization is at the heart of the challenge to develop the new qualification paradigm is overviewed in **Optimization and Uncertainty Quantification**.

Implementation

The development of a new qualification paradigm that is rapid [9], flexible, and practical centers on developing a validated, predictive capability via integrated models in conjunction with real-time in-process and ex-situ diagnostics. The technical challenges that must be overcome to achieve the new paradigm will be discussed in the following sections.

Diagnostics - Process and In-situ

One of the most significant technical gaps is the need for consistent and accurate measurement tools for in-situ diagnostics [10,11]. In-situ measurements are the first step to quantifying and monitoring critical AM process variables for materials control and optimization, and providing correlation to the relevant physics of the process. New and novel measurement techniques, sensors, and correlations to materials science phenomena are needed, and must be well-suited to the spatial, temporal, environmental and processing considerations of AM. Real-time, in-situ measurements are also critical to developing a deep understanding of the AM process, with immediate determination of the impact of a requirement or manufacturing process change, while also allowing for changes in component performance to be quickly diagnosed.

Process control is impeded by a lack of adequate process measurement methods to characterize temperature, geometry, chemistry, phase content, and physical abnormalities, and to quantify and monitor critical AM process variables for materials control and optimization. The highly dynamic nature of some additive processes, e.g. laser powder bed fusion, introduces additional challenges as critical physical events can occur at time scales faster than sensor capabilities and length scales below typical sensor resolutions. Moreover, challenging subsurface measurements are desirable as the voxels continue to evolve and do not reach their metastable end state until they are deeply buried below additional material.

Data management has been observed to be another barrier as high bandwidth process and sensor sets can quickly approach terabytes of data. Ideally, the assessment techniques would be able to define all relevant structure, chemistry, defects, and properties in every voxel of an additively manufactured material, with the goal of connecting all possible variables to part performance. The identification of benchmark process and performance artifacts are vital to materials characterization efforts and testing. Achieving a system that integrates the in-situ and process measurements with these benchmark artifacts would provide designers and process engineers a perfect storm of information for process control.

Assessing Materials and Process Performance

Accurate performance predictions are essential for developing a viable qualification paradigm, and AM provides a range of possible options including uniquely designed benchmark process and performance artifacts, and the use of exemplars to demonstrate efficacy of the approach. These artifacts can be designed to provide accurate validations of performance predictions and monitor process stability. While process and performance artifacts ideally will be identical, it is noteworthy to differentiate between process verification and component performance. Process artifacts (e.g. sacrificial specimens) are typically used to verify process performance through a post-process evaluation. The selection of artifacts for process control and evaluation is a well published subject [12,13] and these efforts are guides to select appropriate performance artifacts.

Performance artifacts in our new qualification paradigm have the goal of verifying component performance in conjunction with in-situ manufacturing diagnostics and predictions of performance. Overall these performance predictions would ideally change the purpose of post-process, product testing to validation rather than performance evaluation. The selection criteria for the performance artifacts are driven by multiple requirements and constraints of AM. First, they must provide the ability to evaluate several material types to assess unique material, design, and process challenges. They should also have modest performance requirements to simplify testing requirements where preferably performance can be assessed by measuring a limited number of requirements, metrics, or properties. These performance artifacts must also be selected considering AM's strengths and shortcomings, such as dimensional tolerances or surface finish, that could dilute the focus from the goal. It also is reasonable to consider applications with an opportunity to evaluate the enhanced functionality of components which can be uniquely enabled by AM.

Rapid Characterization

To succeed in AM material assessment, where properties might vary from voxel-to-voxel or build-to-build, the existing materials assessment paradigm must be modified. Conventional materials assessment typically requires time scales on the order of weeks to months to machine test coupons and prepare for chemical and metallographic microstructural analysis, relying on expensive and time-intensive non-destructive evaluation such as CT scans. The challenge is to create a rapid characterization capability to generate a material assessment in a matter of hours rather than months. A combination of high-throughput, rapid screening characterization techniques with more selective, higher-fidelity assessment of P-S-P-P connectivity using conventional methods is an ideal solution to characterize process variables at the needed spatial and temporal scales. Figure 3 shows a rapid testing configuration [14] where an array of miniature tester bars is produced and tested using AM at a cost and time scale comparable to the testing of a few conventionally produced and tested tensile bars. Having the capability to print and test arrays of tensile bars provides a wealth of data quickly that allows for the capture of the statistical nature of many mechanical properties that is critical to the creation of a new testing paradigm that we refer to as "Properties *Alinstante.*" This testing paradigm requires high-throughput, real-time measurements used in tandem with more detailed, lower throughput measurements to efficiently establish the structure, process, and property relationships of AM materials. Innovative experimental techniques are essential to provide assessment of materials performance and properties, and are required to link the limited information available from *in-situ* information and process and performance artifacts to the full P-S-P-P relationships of real components [15].

(a) (b)

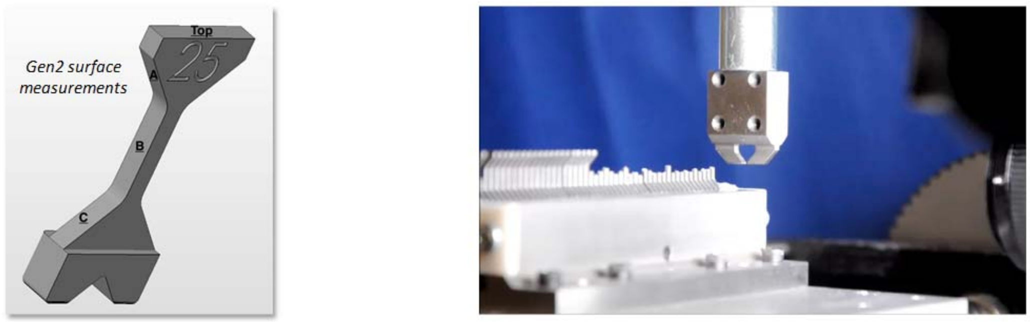

Figure 3: Rapid testing configuration for determining mechanical properties and performance. (a) shows the general mini-tensile bar geometry (b) is a picture of a rapid testing configuration for arrays of AM printed mini-tensile bars

Some quantities of interest in materials assessment are amenable to high-throughput automation and integration (e.g. hardness, chemistry, and electrical conductivity) whereas others (e.g. grain structure, long-term corrosion resistance, thermal diffusivity) are currently not. "Properties *Alinstante"* is required to link the information available *in-situ* (i.e. during processing) with complementary detailed structure and property measurements using conventional techniques to fully establish P-S-P-P relations. To this end, high-fidelity microstructural characterization is required to inform and calibrate multi-scale modeling techniques (including continuum, phase-field and molecular dynamics simulations) to provide microstructural information that can be referenced performance. The ability to predict process and component performance is the first step towards design-by-predictivity.

P-S-P-P Models

A predictive, science-based description of the relevant mechanism responses for the observed properties in AM materials is the end goal for P-S-P-P connectivity. This requires predictive models to be developed using an Integrated Computational Materials Engineering (ICME) [16] approach to achieve fundamental physics-driven design from microstructure to parts and then components. Computational models must relate microstructure to bulk measurable properties to translate AM process results to predictable material properties and ultimately product performance. As such, the structure-property connections in AM materials must encompass the three main length scales: micro-meso material modeling, macro-modeling, and process modeling. Ultimately it is expected that validated computer models will guide the synthesis process, providing a feedback loop for selection of process parameters.

A modeling approach to bridge the length scales is shown in Figure 4 for a metal AM process such as a powder-bed fusion or laser engineered net shaping (LENS) process [17]. The overarching goal of this modeling technique is to eventually achieve finite element analyses of full parts, with accurate thermal histories, microstructures and residual stress fields. Such an approach requires input from all length scales of modeling. We begin with the mesoscale, where discrete element dynamics (DED) simulations are used to study the packing of powder particles [18] as they are spread across the substrate, as in a powder-bed fusion machine. Because the DED simulations have no inherent length scale, it is possible to construct atomistic representations of the particles in the simulated powder pack, to study via molecular dynamics (MD). MD is used to determine the thermal conduction of metals in a powder bed environment, which will give accurate information about the size and shape of the melt pool as a function of laser power and beam width. It is also possible to use these simulations to study changes in melt pool geometry due to oxidization of powders, or powder packs that have skewed size distributions due to powder re-use. Melt pool geometries and thermal conductivities from mesoscale powder and process models are being imported into kinetic Monte Carlo (KMC) simulations, along with thermal histories from macroscale simulations, to develop models of the unique microstructures found in metals subjected to a moving heat source. With accurate microstructures available, microstructurally-aware finite element analysis can be utilized to determine residual stresses in as-built parts [19]. The potential predictive impacts of the models are wide-ranging, and will require iterative loops of experimental characterization and modeling with applied mechanical and thermal stresses to determine feasibility [20]. These models may ultimately identify process routes presently outside the bounds of what is practical or achievable, and guide the design of next-generation AM systems.

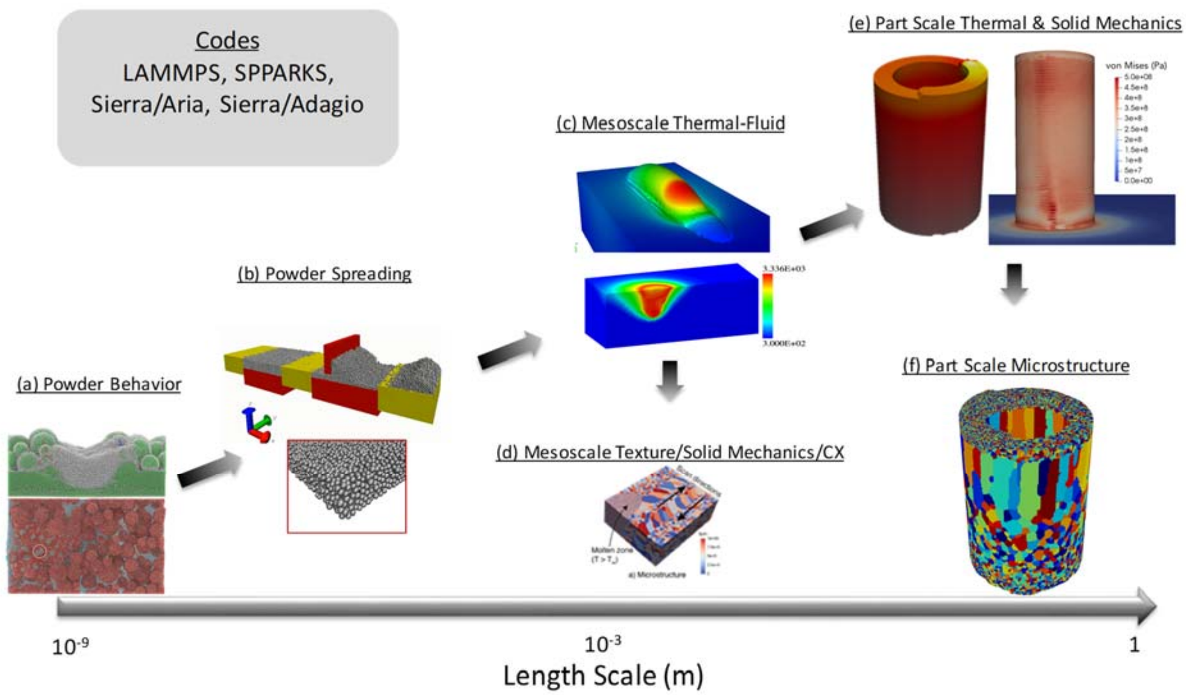

Figure 4: AM process is being simulated at multiple length scales. (a and b) At the powder scale, molecular dynamics and discrete element methods are used to study powder particle flow and physical properties. (c and d) At the mesoscale, combined thermal-fluid simulations provide detailed meltpool information and surface shape. Microstructure simulations also give insight to solidification grain structures. (e and f) At the macroscale, simulations of full parts provide thermal histories and residual stress fields, along with microstructural effects on part performance.

Optimization and Uncertainty Quantification

Ultimately optimization, data science [21,22], and uncertainty quantification [23-26] are at the heart of the challenge. Overall the goals are to (1) use optimization as the interface between simulations, experiments, data, and uncertainties, (2) map numerical capabilities to real experiments, (3) use data science to ask questions, not just answer questions, and (4) use data science in each part of the P-S-P-P map. To provide maximum information and create robust solutions in the face of uncertainties, the development of a research strategy for intelligent data collection and analysis of diverse sources (experiments, diagnostics, models) requires generating, filtering, selecting, and sampling data. To transform practices, we need to be able to characterize uncertainties at all stages: at the raw material stage, during the AM process, in the resulting microstructure of the material created in the AM process, and ultimately, in the product created from that material. These uncertainties are characterized by enormous sets of experimental data, materials models across all length scales, and AM process models. Efficient techniques are needed to propagate parameter uncertainties through models, including sampling, stochastic expansions, interval analysis, and reliability methods. The ability to fully couple numerical multi-scale simulations with efficient analysis tools is necessary so that models can be calibrated, used in an optimal design process, and eventually guide the manufacturing process. Techniques must also be developed and implemented to calibrate model parameters with incorporated experimental uncertainty. Finally, we need to follow structured model validation processes [27,28] for comparing model predictions to experimental data and computing validation metrics under a variety of conditions. Validation helps ensure that each of the models shown in Figure 4 is appropriate for its intended use. This is necessary both for proper use of individual models and for the coupling of models across scales.

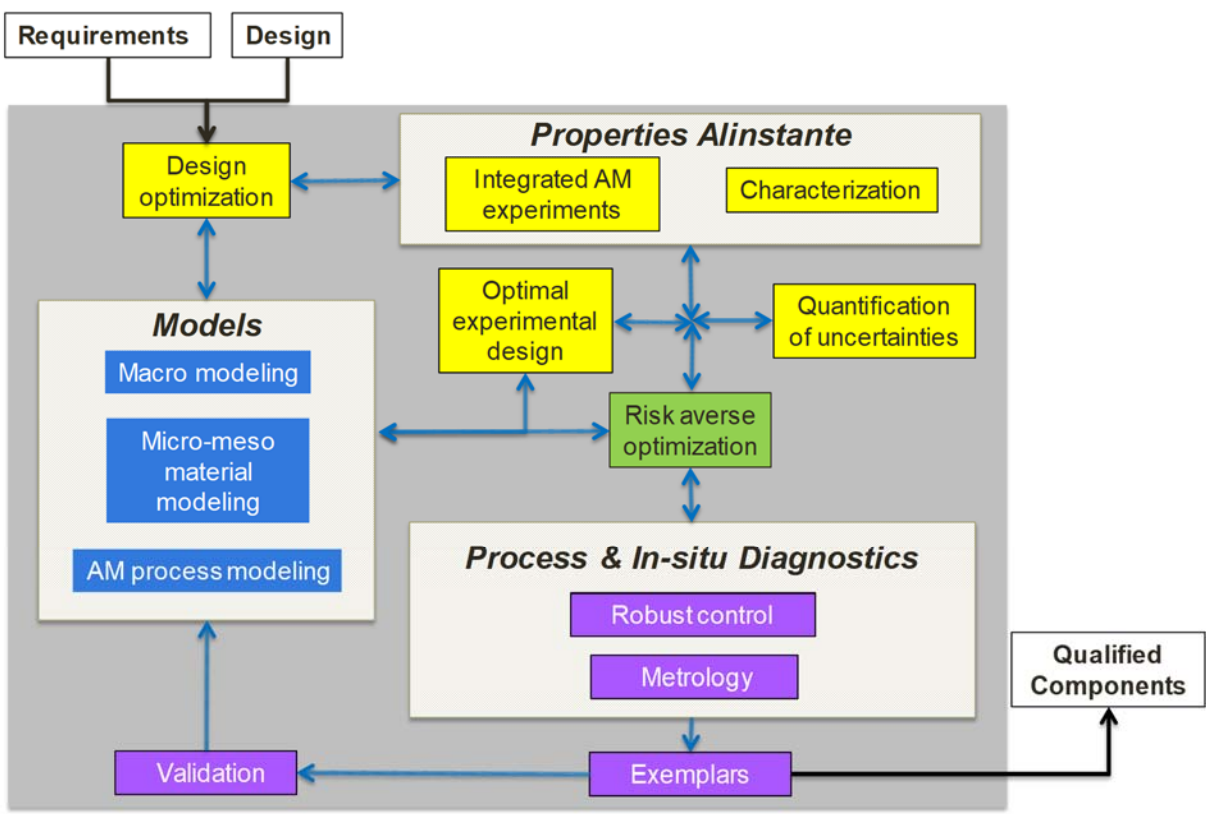

Figure 5: Framework for new AM-driven Qualification Paradigm

Materials characterization, "Properties *Alinstante*", experimental design, integration of AM modeling with micro-meso-macro scale modeling, optimal control, and risk-averse design optimization all play important roles in managing and characterizing uncertainties in the overall product development and qualification. These capabilities drive a possible framework for a new qualification paradigm shown in Figure 5. This new qualification framework utilizes a multi-scale approach that is rapid and flexible where performance is predicted probabilistically and the manufacturing process is tightly controlled. The computational and statistical methodologies exist to achieve end-to-end uncertainty quantification, but the integration with large data sets, many scales of material models, and preliminary AM models makes this task very challenging.

Summary and Conclusions

AM provides the opportunity to develop a new qualification paradigm for materials and components by incorporating deep materials and process understanding. This requires integrating a validated, predictive capability with real-time and ex-situ diagnostics to realize uncertainty quantification driven qualification of design and processes. Success in executing a new qualification paradigm will result in a revolution of component engineering, design, and manufacturing. This new framework, shown in Figure 5, requires integrated models, *in situ* and

process diagnostics, the use of artifacts and exemplars, and uncertainty quantification, all within an optimization focus. Impacts of the new qualification paradigm are far reaching and substantial. Immediate determination of the impact of a requirement or manufacturing process change will be possible with the ability to predict performance of the process, materials and component. The new paradigm will allow for problems or unexpected changes in component performance to be quickly diagnosed and propagated through the design-manufacture-sustainment chain to assess impacts to an entire enterprise. In addition, the ability to verify and predict process stability and eventually materials assurance allows for science-based and trusted manufacturing and an increased confidence in lifetime performance.

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