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Uncertainty Quantification for Additive Manufacturing Process Improvement: Recent Advances

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This paper reviews the state of the art in applying uncertainty quantification (UQ) methods to additive manufacturing (AM). Physics-based as well as data-driven models are increasingly being developed and refined in order to support process optimization and control objectives in AM, in particular to maximize the quality and minimize the variability of the AM product. However, before using these models for decision-making, a fundamental question that needs to be answered is to what degree the models can be trusted, and consider the various uncertainty sources that affect their prediction. Uncertainty quantification (UQ) in AM is not trivial because of the complex multi-physics, multi-scale phenomena in the AM process. This article reviews the literature on UQ methodologies focusing on model uncertainty, discusses the corresponding activities of calibration, verification and validation, and examines their applications reported in the AM literature. The extension of current UQ methodologies to additive manufacturing needs to address multi-physics, multi-scale interactions, increasing presence of data-driven models, high cost of manufacturing, and complexity of measurements. The activities that need to be undertaken in order to implement verification, calibration, and validation for AM are discussed. Literature on using the results of UQ activities towards AM process optimization and control (thus supporting maximization of quality and minimization of variability) is also reviewed. Future research needs both in terms of UQ and decision-making in AM are outlined.

Keywords: additive manufacturing, uncertainty quantification, calibration, verification, validation, process optimization, process control

1 Introduction

Additive manufacturing (AM) is a revolutionary technology for manufacturing products with complex geometry without wasting much material in comparison to traditional manufacturing techniques. However, several factors such as cost, production volume, energy consumption, material property requirements, labor requirements, market competitiveness, sustainability, etc. affect the adoption of this technology. One major factor inhibiting the widespread implementation of AM is the challenge in certifying additively manufactured products due the variability in product quality. Since physical experiments are expensive, a digital representation of the AM process in the form of models (computational models based on physics and machine learning models based on experimental data) provide an attractive alternative to study the variability in the quantity of interest (QoI) of an AM product (such as geometric accuracy, porosity, residual stress or strength), and to support process optimization and control decisions to improve the quality of the product. AM is a complicated process with multiple physics at multiple spatial and temporal scales; therefore multiple physics-based models are needed to describe the various components of the process. Since no model can accurately represent the physical process, there are several sources of uncertainty in each of these physics-based models. There are also uncertainties in experimental setup, measurements, data processing algorithm, etc. which introduce uncertainty in the prediction of machine learning (ML) models that are built using experimental data. For decisions on AM process improvement – such as process design, process control, and resource allocation – based on AM models to be effective, it is necessary to take into account the various sources of uncertainty in the AM process and models, and update the uncertainty information as more data becomes available in real-time [1].

In AM, uncertainties regarding process inputs (laser velocity, temperature, etc.), model parameters (thermal properties, mechanical properties, etc.), and various types of model errors lead to uncertainty in the model prediction. Three types of activities address *model uncertainty*: (a) Calibration, (b) Verification, and (c) Validation. *Model calibration* is the process of estimating the values of model parameters (and model discrepancy) based on experimental data. In other words, model calibration is the tuning of the unknown model parameters and discrepancy that cannot be directly measured using experiments. *Model verification* is "the process of determining that a model or simulation implementation and its associated data accurately represent the developer's conceptual and mathematical description and specifications" [2]. In practical terms, this activity results in the identification of coding errors and quantification of numerical errors in the implementation of a physics-based model (e.g., discretization error in a finite element model, truncation error in a reduced-order model, and surrogate model error when a detailed physics model is replaced by an inexpensive surrogate model). *Model validation*, on the other hand, is "the process of determining the degree to which a model or a simulation is an accurate representation of the real world from the perspective of the intended uses of the model or the simulation" [3]. In practical terms, this activity involves comparing model prediction against real world observation and computation of a validation or error metric that evaluates the agreement between prediction and observation. Uncertainty quantification (UQ) consists of both forward and inverse problems; in the *forward problem*, the various uncertainty sources are propagated through the system model to quantify the uncertainty in the model prediction; whereas in the *inverse problem*, the model parameters and discrepancy are estimated based on the comparison of model prediction and real-world observation. The acronym VVUQ (verification,

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validation and uncertainty quantification) is also being used to describe the collection of the activities and analyses described above (e.g., ASME Journal of Verification, Validation and Uncertainty Quantification, and ASME Committee on Verification, Validation and Uncertainty Quantification, and its subcommittees).

In UQ, there needs to be explicit recognition and quantification of both aleatory and epistemic sources of uncertainty; aleatory uncertainty refers to the natural variability of physical quantities, whereas epistemic uncertainty refers to lack of knowledge, arising from data uncertainty (e.g., sparseness, imprecision, omissions, and measurement and processing errors) and model uncertainty (unknown model parameters, numerical errors, and model form errors). Some of the model inputs (laser power, laser velocity, etc.) and model parameters (thermal properties, mechanical properties, etc.) can have both aleatory and epistemic uncertainty, (i.e., variability across different AM runs as well as unknown actual value in any one run). In such cases, it is also desirable to separate the contributions of aleatory and epistemic uncertainties, in order to have clear interpretability of model validation and UQ results [4], and to support decision-making for uncertainty reduction (i.e., model refinement vs. additional experiments) by identifying the dominant uncertainty sources through sensitivity analysis [5, 6].

Research on appropriate techniques for verification, validation, calibration, and uncertainty quantification in AM is in its beginning stages at present. Until recently, these methods have been mainly studied for models of physical systems involving individual physics disciplines (such as solid mechanics, fluid mechanics, and heat transfer), and have been geared towards quantifying the model errors and prediction uncertainty of physics-based models. The extension of these methodologies to additive manufacturing has to address multi-physics, multi-scale interactions.

Manufacturing of any product typically goes through multiple processes, each with different physics and phase transformations over space and time. For some of the manufacturing processes, physics-based or mechanistic models are not available; in such cases, data-driven empirical models are developed for prediction purposes. The extension of VVUQ methods to such data-driven models is a current topic of research.

AM is a very young and rapidly advancing area even within the field of manufacturing. AM includes several different types of technologies, all of which are under active study and improvement. The technologies address different types of materials, such as metals, plastics and composites. However, the products of AM are found to have significant variability in geometric accuracy, roughness, strength properties, and flaws such as porosity, delamination etc. Many researchers in industry, government and academia are actively studying approaches to reduce the variability and improve the AM product quality, and are also studying appropriate measurement techniques for AM products including online monitoring.

Several organizations have been developing standards and guidance documents for UQ-related methods and activities (e.g., DOD [2], NASA [3], ASME [7–10], AIAA [11], ASTM [12, 13], ISO [14–17], IEEE [18], and TMS [19]). There is also a significant body of literature and standards regarding software quality and data quality. However, attempts to extend these approaches and methods to manufacturing processes, especially additive manufacturing, are only beginning now. For example, the ASME Standards Committee on Verification, Validation and Uncertainty Quantification in Computational Modeling and Simulation has a subcommittee on advanced manufacturing, which is making efforts to develop guidance regarding the extension of UQ and V&V methods to manufacturing processes including additive manufacturing. Another recent effort is the formation of an industry/government/academia steering group Computational Materials for Qualification and Certification (CM4QC), particularly focused on AM and addressing UQ and V&V needs for AM process models.

The issues, challenges and activities discussed above provide the motivation and context for survey the state of the art in the application of UQ and V&V techniques to AM. This paper reviews recent research literature in UQ and V&V techniques for AM and their use in process optimization and control.The scope of the paper is restricted to review of the research literature; we do not intend to demonstrate the methods, develop new approaches, or present case studies in this paper. The remainder of the paper is organized as follows. Section 2 provides a brief introduction to AM techniques and process models, and Section 3 briefly discusses the uncertainty sources in the AM process models. Sections 4, 5 & 6 survey the literature on methods related to quantifying model uncertainty (calibration, verification and validation) and challenges in applying these methods to AM process models. Uncertainty aggregation from multiple sources and activities is discussed in Section 7, addressing the multi-physics, multi-scale interactions in the AM process. Literature on process optimization and control incorporating UQ results is provided in Section 8. In Section 9 ideas for implementing UQ in AM are discussed. Section 10 provides the concluding remarks.

2 AM processes and models

AM, also commonly known as 3D printing, is the process of manufacturing parts by adding material in layers. Traditional manufacturing techniques such as subtractive, casting, forging, etc. based on removing, joining, or shaping material work well with mass production of parts with simple geometry. AM, on the other hand, is particularly advantageous for manufacturing parts with complex intricate geometry in lower quantities [20], but is also being employed for mass production [21]. The part geometry is defined in a computer-aided-design (CAD) software, and the resulting .stl (stereolithography) file provides the slicing and laser path information to the printer for manufacturing the AM part. The sensors (thermal camera to monitor temperature, profiliometer to monitor surface roughness, etc.) monitor the manufacturing process and the master controller controls the material deposition and the laser. Figure 1 shows the schematic of one type of AM process, namely directed energy desposition, as an example. Based on the type of material (metallic, ceramic, polymer or composite) and technique used to create the layers, ASTM [12] classifies AM processes into seven categories as follows [22–25]:

(1) Vat photopolymerization [26]: A light source (ultra-violet radiation) cures liquid photopolymers in a vat to manufacture parts. It is the first industrial AM technology.
(2) Material extrusion [27]: Filaments of material are melted using a heated nozzle to create a 3D part. This is one of the most popular and accessible AM technologies.
(3) Powder bed fusion (PBF) [28]: A bed of raw material in powder form is melted or partially melted using lasers or electron beams to produce parts in the desired shape. This is a very popular AM technology.
(4) Directed energy deposition (DED) [29]: A focused energy source such as laser, electron beam, or arc plasma fuses material as they are being deposited to manufacture the AM part. This is similar to material extrusion and can be used with a variety of materials.
(5) Binder jetting [30]: Powdered raw material is joined together using a liquid bonding agent to form the part. Unlike other AM processes, this process does not employ heating to fuse the material.
(6) Material jetting [31]: Droplets of material are selectively jetted and cured by ultra-violet light to form the part. This technique is similar to common inkjet printers in 3D.
(7) Sheet lamination [32]: Thin sheets of material are stacked and laminated together using adhesives, ultrasonic welding, brazing, etc. It is a cheap and fast process, making it ideal for low-fidelity prototyping [23].

Table 1 summarizes the AM processes and the different technologies, the form of the raw material used, and the suitability of the material with process [33, 34].

All the AM processes, irrespective of category, technology, or material, follow the basic principle of layer-wise addition and fu-

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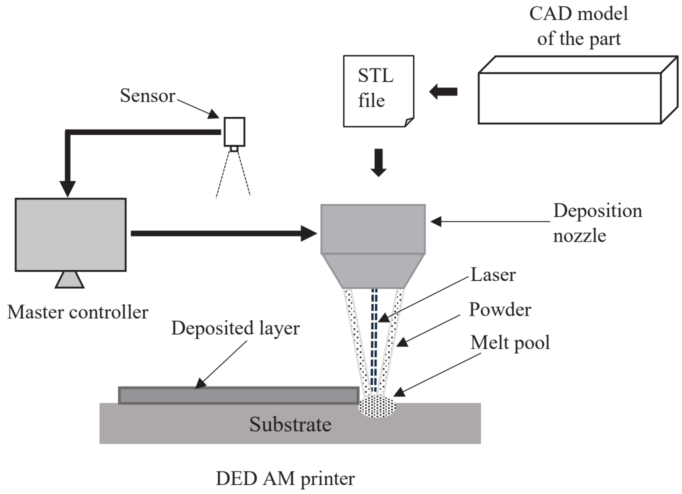

Fig. 1 Schematics of the directed energy deposition AM process

sion of material. Using the DED AM process as an example, it can be seen in Figure 1 that manufacturing an AM part is complicated. Interaction between the heat source (laser) and the raw material (powder) may vary from layer-to-layer and from one location to another within a layer. Other AM processes also have similar complicated material addition and fusion phenomena to manufacture the part. In contrast to traditional manufacturing, AM parts may not be homogeneous and may show substantial variation of properties across samples and also spatially. This variability, inherent to the process and the parts, is *aleatory uncertainty*. In the past, attempts have been made to understand the AM process using trial-and-error experimental approaches. Recently, the shift has been towards using computational models in support of process optimization, and physics-based and data-driven models are both being developed for various steps in the AM process.

Due to the complex physics involved in the AM process and the multi-level characteristics, physics-based AM process simulation usually involves multiple simulation techniques connected in a multi-level manner. The laser-based process used for metals is described by the following physics-based models: powder stream model, heat source model, melt pool model, solidification model, and residual stress model as shown in Figure 2. The powder is deposited layer upon layer and is melted by the laser traveling in a predefined path. The output of the laser heating process and powder bed forming process are then used as inputs to the melt pool model. The outputs of the melt pool model are then employed as inputs to the solidification model. From the solidification model, the solidified microstructure is simulated and finally used as input to the macro-level mechanical properties analysis (Figure 3).

Various simulation techniques have been developed to enable the multi-physics and multi-scale AM process simulations using commercial software and in-house codes. For instance, discrete element methods have been widely employed to develop the raindrop model for powder bed forming [36], computational fluid dynamics (CFD) models have been used for fluid flow modeling of melt pool [37–43], finite element models (FEM) have been developed to perform thermal and residual stress analyses [44–49], phase-field and cellular automata models are used for solidification microstructure evolution modeling [50–53], and crystal plasticity model is used for mechanical and fatigue properties prediction [54]. Ye et al. [55] proposed a crystal plasticity framework to study fatigue behaviour in AM parts based on the microstructure. Wang et al. [56] coupled finite element and phase field models for laser-based welding, a process not different from direct energy deposition in AM, in order to simulate grain growth in the molten pool. Guan and Zhao [57] reviewed the analytical, numerical, and hybrid modeling approaches of the DED process. Several literature reviews on the AM process modeling approaches have been published in recent years [27, 34, 58–61].

Several other studies have focused on developing data-driven machine learning (ML) models for the AM processes, based on experimental data. Data-driven models are considered to have an advantage over physics-based since real-world behavior in actual experiments is used in model construction [62]. Khanzadeh et al. [63] compared the performance of several supervised ML algorithms (decision tree, k-nearest neighbor, support vector machine, linear discriminant analysis, and quadratic discriminant analysis) in detecting porosity using melt pool thermal images. Sharma et al. [64] built an artificial neural network (ANN) model using data published in the literature to study the influence of AM process parameters and post-fabrication parameters on the tensile properties of the AM parts. Extreme gradient boosting (XGBoost) and long short-term memory (LSTM) were employed to predict melt pool temperature in AM DED process and the accuracy and performance of the models compared [62]. Nalajam and Varadarajan [65] proposed a hybrid model to forecast layer-wise melt pool temperature by combining long short-term memory (LSTM) with convolutional neural networks (CNN). Srinivasan et al. [66] used a combination of ML techniques such as symbolic aggregate approximation (SAX), principal component analysis (PCA), and density-based spatial clustering of applications with noise (DBSCAN) to search the process parameter space to produce complex AM parts with a more homogeneous thermal history. Zhang et al. [67] studied improvement in defect detection using flash thermography in AM by proposing novel ML methods (spatial–temporal blind source separation (STBSS) and spatial–temporal sparse dictionary learning (STSDL)) for separation of noise from signal in thermography images. Jin et all. [68] in their review of data-driven techniques in AM categorized them under three main stages of AM viz., geometrical design (i.e., topology optimization), process parameter configuration, and anomaly detection. Tian et al. [69] reviewed the recent progress in data-driven AM models from the perspectives of material design, structure design, and tool path planning. Comprehensive reviews of the application of various types of ML techniques in AM are available in Refs. [70, 71]. One challenge for ML models is the requirement of large amount of training data; this may be unaffordable given the high cost of the AM process. Another challenge is that if the ML model is built purely on experimental data, it may not be consistent with the constraints of actual physics of the process. Therefore, several studies [72–74] have investigated several physics-informed machine learning (PIML) approaches to build AM process models (e.g.,

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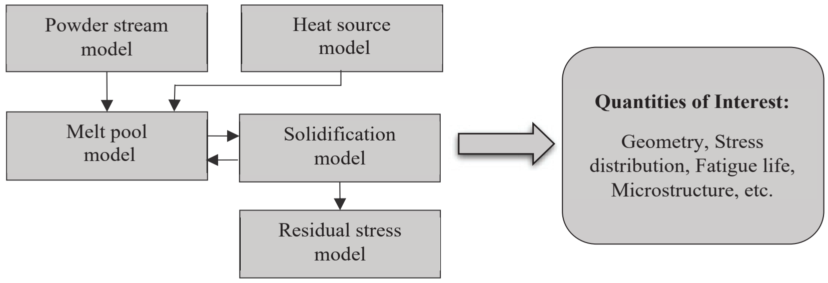

Fig. 2 Physics-models for laser-based AM process [35]

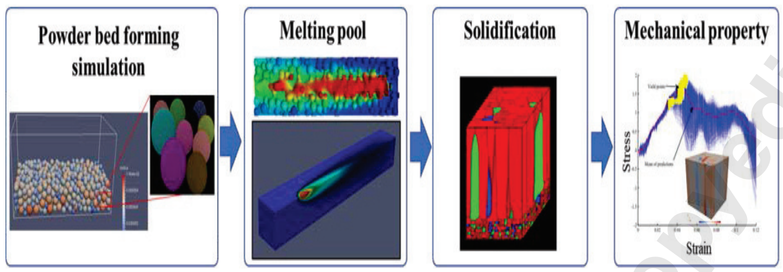

Fig. 3 AM process simulation: multiple physics and scales

Gaussian process, deep neural network (DNN), and recurrent neural network (RNN) models) by combining both physics knowledge (either physics-based models or simply physics constraints) and experimental data; the PIML strategies help to address the challenges of physical inconsistency as well as data scarcity.

3 Uncertainty in AM process models

Both physics-based and data-driven AM process models have several sources of aleatory and epistemic uncertainties [35]. These are discussed in this section.

3.1 Uncertainty sources. *Model parameter uncertainty* arises from lack of knowledge (epistemic) regarding the correct values of the model parameters in printing a particular part. In the case of AM, since the manufacturing process happens in high temperature, the material properties such as density, conductivity, specific heat etc. (which are model parameters) are temperature dependent and show non-monotonic behaviour [75]. The properties of the substrate are sometimes different from the properties of the feed powder. In addition, these parameters may have inherent variability from one part to another which is aleatory uncertainty. Thus calibration of the material parameters is necessary to obtain an accurate simulation model.

Input uncertainty relates to the values of the process settings (such as laser power and velocity) that need to be used as inputs to the AM process simulation model. Several models are available for the laser heat source [76–79] to study the heat density elongation due to the fast movement of laser on the material deposit. Mirkoohi et al. [79] studied the effect of laser-matter interaction using five different types of heat sources - steady state moving point heat source, transient moving point heat source, semi-elliptical moving heat source, double elliptical moving heat source, and uniform moving heat source. However, the parameters of the heat source have to be calibrated [76] to best represent the physical process, which is challenging given the various sources of uncertainty in the experimental measurements. In addition, the value of a process parameter (e.g., temperature) may be different from the value reported by the sensor. Thus, both aleatory and epistemic uncertainty are encountered in characterizing the AM process inputs.

Model uncertainty: The physics-based models have several assumptions and simplifications regarding the physical phenomena in the AM process (e.g., laser shape, heat transfer mechanism, grain nucleation and grain growth mechanisms, etc.), causing *model form error*; this type of error is addressed by model validation in general (but also in calibration when a model discrepancy term is estimated). Further, numerical approximation error is caused while solving the numerical model, giving rise to errors such as discretization error, truncation error, round-off error, etc.; these types of errors are addressed by model verification. Two recent reviews in the literature discuss uncertainty quantification needs and challenges in the context of physics-based AM process models [1, 80]. A systematic approach for uncertainty quantification by considering the errors and parameter uncertainties in different components of physics-based AM models and their propagation to the variability in grain morphology is outlined in [35]. A small number of UQ studies are reported on UQ for a chain of models [81, 82]; physics-based modeling of the AM process consists of multiple models (at different physics and scales). In the case of data-driven machine learning (ML) models for AM processes, the model parameters are estimated from experimental data. Measurement errors, input uncertainty, and limited amount of training data (i.e., number of experiments) lead to uncertainty in the parameter estimation and therefore the prediction of the data-driven model. Meng et al. [70] identify UQ in ML models for AM as one of the future research directions. Methods for uncertainty quantification in the prediction of both basic ML models and physics-informed ML models in AM were studied in [73, 74]; this work also implemented stochastic sensitivity analysis with these ML and PIML models to compare the contributions of different uncertainty sources to the model prediction uncertainty.

3.2 Model uncertainty quantification. Figure 4 shows the various stages of UQ in AM. This section focuses on the third stage, *model uncertainty quantification*, which consists of the following activities: calibration, verification, validation, and uncertainty aggregation. Note that in verification occurs before calibration in Figure 4. This is a desirable sequence. Verification can be first used to compute the numerical errors in the model; next, these numerical errors can be accounted for during the model calibration, so that model parameter estimation is not confounded by the numerical errors [83].

Consider a model $G(\boldsymbol{X}, \boldsymbol{\theta})$ with controllable inputs $\boldsymbol{X}$ and

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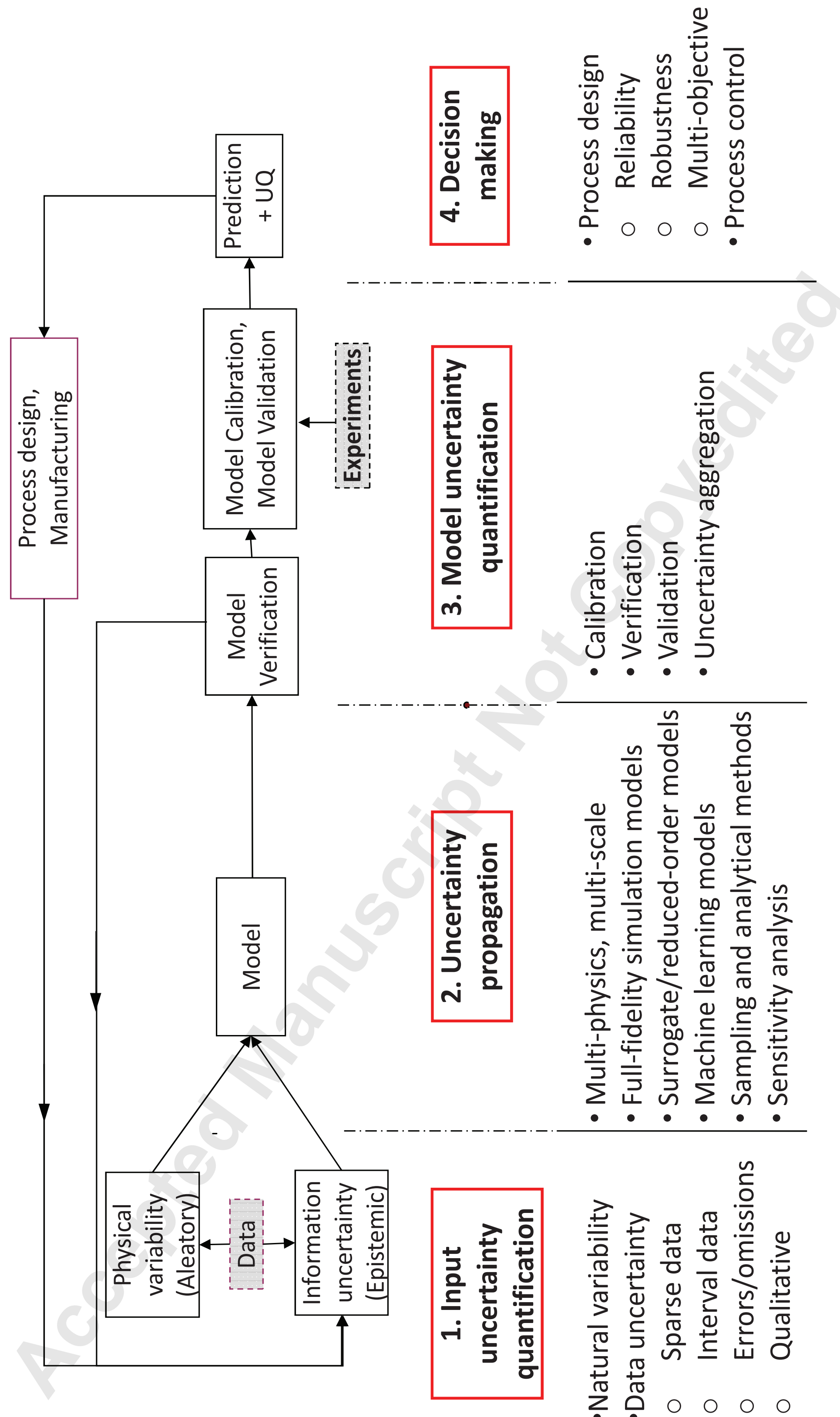

Fig. 4 UQ flowchart

model parameters $\boldsymbol{\theta}$. The model parameters are uncontrollable, and are not directly measured; rather, they have to be inferred based on the experimental observation of the input and the output.

The relationship between the model prediction (y_m), experimental observation y_{obs}, and actual value (y_{true}) of the output quantity of interest (QOI) can be conceptually expressed as

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Table 1 AM processes categories [33, 34].

AM category	Technologies	Raw material form	Material type
Vat photopolymerization	Stereolithography (SLA), Direct Light Processing (DLP), Continuous Direct Light Processing (CDLP)	Liquid	Polymers, Ceramics
Material extrusion	Fused Filament Fabrication, Robocasting	Solid	Polymers, Composites
Powder bed fusion	Selective Laser Sintering (SLS), Selective Laser Melting (SLM), Electron Beam Melting (EBM), Direct Metal Laser Sintering (DMLS)	Powder	Metals, Polymers, Ceramics, Composites, Hybrid
Directed energy deposition	Laser Engineered Net Shape (LENS), Electron Beam Additive Manufacture (EBAM)	Powder, Solid	Metal, Hybrid
Binder jetting	3D inkjet technology	Powder	Ceramic
Material jetting	Three-dimensional printing (3DP), Inkjet printing (IJP), Multijet modelling (MJM), Ballistic particle manufacturing (BPM), Thermojet	Liquid	Polymers Metals Ceramics Composites Hybrid
Sheet lamination	Laminated Object Manufacturing (LOM), Ultrasonic Additive Manufacturing (UAM), Selective Deposition Lamination (SDL)	Powder	Polymers, Ceramics Metals Hybrid

$$y_{obs} = y_{true} + \varepsilon_{obs} \tag{1}$$

$$y_{true} = y_m + \varepsilon_{mf} \tag{2}$$

where ε_{obs} and ε_{mf} are observation error and model form error respectively, if there are no numerical errors in the model prediction. Combining Eq. 1 & Eq. 2,

$$y_{obs} = y_m + \varepsilon_{mf} + \varepsilon_{obs} \tag{3}$$

In practice, the model prediction (y_m) is obtained using numerical computation (e.g., FEA, CFD etc.); thus (y_m) consists of the numerical solution (y_{nm}) of the model G and the solution approximation error (ε_{nm}):

$$y_m = y_{nm} + \varepsilon_{nm} \tag{4}$$

These equations are only notional, and the exact way the errors combine might be more complicated. The aggregation of these errors is non-trivial and needs to follow a systematic procedure. Sankararaman et al. [84] showed that a Bayesian network approach provides an efficient and accurate method for combining the errors.

The first step in model uncertainty quantification is model verification, which identifies coding implementation errors and quantifies the numerical solution approximation error (ε_{nm}). This is followed by model calibration, which estimates the model parameters (and model discrepancy due to model form error) based on calibration experiments. Then, during model validation, the calibrated model needs to be validated with additional data that is not used in calibration. The state of the art in the implementation of these three activities for AM process models is surveyed in the next three sections.

4 Model Verification

Analytical solutions are generally not available for the complicated physical phenomena in AM processes. Thus, several approximate numerical techniques such as FEA, CFD and heat transfer analysis are used. These methods invariably have solution approximation errors such as discretization errors, truncation errors, round off errors, etc. In addition, there are coding errors in the computer implementation of the physics model. Systematic procedures have been developed in the UQ literature for model verification to identify coding errors and quantify numerical errors [85]. The literature on numerical error quantification in AM process models is reviewed below.

Consider the discretization error in finite element (FE) solutions in the context of computing the residual stress in a part manufactured by the EBM process. Computation of residual stress would require thermo-mechanical analysis employing first a heat transfer model whose output becomes the input to a mechanical stress analysis model [86]. Figure 5b shows the heat contour from the heat transfer analysis with a Gaussian heat source for a single scan analysis. The result from the FE analysis (for any discretization-based computational method) depends on the mesh size. The discretization error is often quantified using Richardson's extrapolation [87] using coarse, medium and fine meshes. However if the change in the output with mesh size is not monotonic, Richardson's extrapolation is not applicable.

To handle this limitation of Richardson's extrapolation, Rangavajhala et al. [88] proposed the construction of a Gaussian process (GP) model trained with model predictions corresponding to different mesh sizes. This GP model is used to estimate the corrected model output at a very small mesh size (≈ 0). However, this technique requires FE model evaluation at different mesh sizes and can be expensive. At coarser mesh sizes, the FE solution may not converge, and at finer mesh sizes the simulation time

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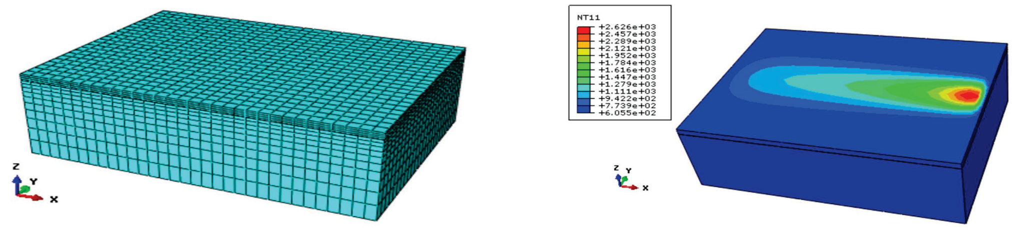

(a) Part mesh (b) Temperature contours

Fig. 5 Heat transfer analysis in the EBM process. See [86] for details.

may be very long. In the case of FE analysis of laser-based AM, a non-uniform meshing strategy is generally employed for computational efficiency [53]; a finer mesh is employed for the powder layer where the laser heat flux is applied and the mesh gradually coarsened away the region of high flux as shown in Figure 5a. The aspect ratio of the mesh elements also needs to maintained carefully for each element and not varied too much in the neighborhood of the location of interest for the mesh to be of good quality and to avoid element distortions. This makes the application of these techniques cumbersome.

Adaptive meshing is a popular technique in AM models. In the FE-based thermo-mechanical analysis of AM processes, for stable solution in the presence of high non-linearity the mesh size needs to be very fine at the thermo-mechanical affected zone (TMAZ) [89]. However, such a fine mesh on the entire path causes unaffordable computational burden. Thus, Baiges et al. [89] presented an adaptive meshing strategy to coarsen the mesh away from TMAZ and to account for the error caused by this coarsening, by introducing two correction terms. Olleak and Xi [90] used an adpative remeshing techinque to reduce the computational effort in predicting distortions in the AM part. The reduction in computational time is achieved by using finer mesh at layers being built that have high temperature and stress gradients. This strategy may not be available for researchers using commercially available FE software as a black box. Another study proposed an efficient adaptive remeshing technique that enables part-scale SLM process simulations and helps reduce model size without sacrificing accuracy [91]. Unlike Richardson's extrapolation method that gives a corrective term to be added to the results from any mesh size, the adaptive meshing techniques attempt to make the discretization error negligible and rely on the convergence of the analysis; thus they may require a few trials to arrive at the optimum simulation parameters.

In addition to the above, several approaches have been explored in the literature for the verification of AM computational models for individual physics such as thermal/melt pool model, solidification model, residual stress model, etc. Schwalbach et al. [92] developed a fast-acting Discrete Source Model to predict the melt pool in powder bed fusion (PBF) AM. They verified the developed model by investigating impact of various physical and numerical approximations and reproducing a known analytical solution for melt pool dimensions in the case of a laser beam moving at uniform velocity. In an effort to verify models describing melt pool behavior, Mindt et al. [93] performed a code-to-code verification for the cooling rate of melt pool calculated using two different methods including Lattice Boltzmann and Finite Volume Computational Fluid Dynamics. Similarly, Harley et al. [94] conducted a code-to-code verification between two thermal models including a model developed in commercial software and a model developed using the finite volume method. Both models are investigated for mesh independence. Mooney et al. [95] verified the accuracy of a thermal model developed based on the Nucleation Progenitor Function approach. Mooney and McFadden [96] performed a verification study for the Bridgman Furnace Front Tracking Model, which is a model used to predict the crystal growth based on the temperature gradient. In their verification study, the simulation model was adopted for a pristine material and then compared against an analytical solution of the same process under the same processing conditions. Pineau et al. [97] conducted a code-to-code verification for phase field and cellular automata methods, which are two widely used solidification models. Seredyński verified the 2D Bridgman model for grain growth prediction [98], by comparing the prediction with ANSYS Fluent solutions [99]. Krol et al. [100] proposed a method to verify the numerical accuracy of the residual stress state using neutron diffraction. The predicted residual stress states of additively manufactured parts were verified by adjusting the support design and using neutron diffraction.

Verification methods in AM have mostly considered only single-physics models, such as solid mechanics, fluid mechanics or heat transfer individually. Due to the presence of coupled multi-physics models, AM models need sophisticated strategies for numerical error estimation (and thus verification) in coupled physics-based models. Rangavajhala [88] developed a novel strategy for discretization error estimation when different meshes are employed for different phases (e.g., solid and fluid), while also considering mesh mismatch between two phases. Further research on the estimation of other numerical errors is needed for AM process models, including verification of high-dimensional response.

5 Model Calibration

After model verification, the model parameters and model discrepancy (due to model form error) need to be estimated using experimental data, for physics-based AM models. Several approaches can be employed to calibrate model parameters such as linear and nonlinear least-squares regression [101] and maximum likelihood estimation [102] for point estimates of the model parameters, and Bayesian calibration [103] to obtain the posterior distribution of the model parameters, where the prior distribution is assumed based on available information. Kennedy and O'Hagan extended the Bayesian approach to incorporate various sources of uncertainty including measurement error and model discrepancy. Recent studies in Bayesian model calibration use the Kennedy and O'Hagan framework (KOH framework) [104], and estimate the model discrepancy term along with the model parameters. Following the KOH framework, Eq. 3 can be re-written as

$$\boldsymbol{y}_{obs} = \boldsymbol{y}_m(\boldsymbol{X}, \boldsymbol{\theta}) + \delta(\boldsymbol{X}, \boldsymbol{\theta}_\delta) + \boldsymbol{\varepsilon}_{obs} \tag{5}$$

where $\delta(\boldsymbol{X}, \boldsymbol{\theta}_\delta)$ is the model discrepancy term to account for the effect of model form error, and $\boldsymbol{\theta}_\delta$ are the parameters of the model discrepancy term. The observation error is generally represented by a Gaussian distribution with zero mean and σ_{obs} standard deviation. Model calibration in the KOH framework involves calibrating the quantities $\boldsymbol{\Theta} = [\boldsymbol{\theta}, \boldsymbol{\theta}_\delta, \sigma_{obs}]$. Using Bayes' theorem, the joint posterior distribution of the calibration quantities $\boldsymbol{\Theta}$ is obtained as

$$f(\boldsymbol{\Theta}|\boldsymbol{y}_{obs}) = \frac{f(\boldsymbol{y}_{obs}|\boldsymbol{\Theta}) f(\boldsymbol{\Theta})}{\int f(\boldsymbol{y}_{obs}|\boldsymbol{\Theta}) f(\boldsymbol{\Theta}) d\Theta} \tag{6}$$

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where $f(\mathbf{\Theta})$, $f(\mathbf{y}_{obs}|\mathbf{\Theta})$, and $f(\mathbf{\Theta}|\mathbf{y}_{obs})$ are the joint probability density function (PDF) of Θ, likelihood function, and the joint posterior PDF. In the absence of an analytical solution, sampling-based methods such as Markov chain Monte Carlo (MCMC) method are usually employed to obtain the posterior distribution. Since MCMC sampling requires thousands of model runs, the expensive physics-based AM models are replaced by inexpensive surrogate models constructed using techniques such as Gaussian process (GP) modeling or Kriging, polynomial chaos expansion, artificial neural networks, etc. In that case, the surrogate model error introduced by the surrogate model also needs to be estimated. Kapusuzoglu et al. [105] implemented the above approach for fused filament fabrication AM using a Gaussian process surrogate model for the physics model, as well as a Gaussian process model for the discrepancy term. Construction of a surrogate model requires multiple training runs of the original physics model, which might be prohibitive if the physics model is computationally expensive. In that case, a low-dimensional surrogate model might be considered with a subset of the parameters that are likely to be most important (see below).

The choice of parameters to be calibrated is dependent on experimental and computational resources. Bruna-Rosso et al. [76] estimated the parameters of the Goldak heat source from the empirical relationship between melt pool geometry and heat source parameters; uncertainty was not considered in this work. Mahmoudi et al. [106] replaced the heat transfer AM model with a GP surrogate model to calibrate the model parameters: powder porosity, laser absorptivity, and coefficient of thermal conductivity. When computational resources are limited, construction of a surrogate model with all the model parameters $\boldsymbol{\theta}$ may not be feasible. Then the discrepancy term in Eq. 5 is considered to represent the uncertainty from all the sources, and is the only term to be calibrated [107]. A common problem with calibration with the KOH framework is the problem of identifiability [108], i.e., it is difficult to distinguish between the effects of model parameters, discrepancy term, and observation error (Eq. 5), especially in the presence of limited calibration experiments. Arendt et al. [109] proposed using multiple responses to calibrate a common set of calibration parameters to improve identifiability. The effectiveness of this approach depends on the characteristics of the responses being used for calibration. Other strategies to improve identifiability are employing Global Sensitivity Analysis (GSA) to identify the most sensitive parameters and only calibrating them; and ignoring the discrepancy term during the calibration step and subsequently building a separate surrogate model for the discrepancy term [105].

In the case of AM models, inputs and/or outputs to the surrogate model can be high-dimensional. Thus, several studies have employed dimension reduction techniques (such as singular value decomposition or principal component analysis for output dimension reduction and GSA and active subspace discovery for input dimension reduction) before constructing the surrogate models for the AM process models [35, 86, 110, 111]. These efficient surrogate models can then be used to calibrate the model parameters [112] using MCMC sampling.

High dimensional outputs also pose a challenge in the design of manufacturing experiments for parameter calibration. Randomly selecting the spatio-temporal locations for experimental measurement runs the risk of obtaining unimportant information, whereas using a large number of locations for measurement makes the measurement infeasible and the calibration computations expensive. Therefore sensor placement optimization techniques to efficiently select the optimal measurement locations for maximizing the information gain in model calibration have been developed [113, 114]. Similar approaches can be investigated for use in AM, in order to achieve balance between experimental effort, computational cost, and effective model calibration.

Existing studies on AM model calibration have considered the parameters to be constant and do not account for variability over space and time, or across specimens. Methodologies developed in other fields to handle the calibration of spatially varying parameters such as a multi-resolution strategy [115], and random field modeling (using Karhunen-Loeve expansion and polynomial chaos expansion) [113] may be adapted to consider such variability in AM.

AM models for predicting the output quantity of interest (QoI) are available at different levels of fidelity. For example, several models and numerical solution strategies are available to predict the melt pool geometry with varying degrees of accuracy such as analytical equation, FE model, CFD model, etc. Generally, a more accurate model is also computationally more expensive [116]. Multi-fidelity model fusion strategies for model calibration are available in the literature [114, 117] by correcting the lower-fidelity model first with the higher fidelity model prediction and then with experimental data in the context of dynamics model. Combining models of different fidelity into a multi-fidelity model can significantly reduce the computational cost in calibration without sacrificing accuracy in AM models.

As seen in Figure 2, the suite of models required to represent an AM process are based on different physics and have complicated couplings between them. The calibration of model parameters in this situation is not straightforward. Simultaneous Bayesion calibration of all the model parameters can be prohibitively expensive. DeCarlo et al. [82] developed a segmented calibration approach for multi-physics (aero-thermal) models considering model dependence and data availability. Extension of such methodologies to AM models could help reduce the computational expense of calibrating coupled multi-physics AM models.

6 Model Validation

Validation involves the comparison of model prediction against real-world observation; however, both prediction and observation are uncertain quantities, as discussed in Section 3. Note that the model validation is done after the model verification (Section 4) and model calibration (Section 5) steps. Thus, ideally in the model validation step a verified and calibrated model is compared against experiments. The experimental data used for model validation should be different from the experimental data used for model calibration.

When the AM process model is used for decision-making such as process parameter optimization, validation can be carried out at two stages: (1) Validation of physics model prediction of the quantity of interest (QoI) by quantifying the difference between the model prediction and experimental observation [118] or by computing various validation metrics [119] mentioned in this section (Section 6). (2) Validation of model-based decision such as process parameter optimization by conducting experiments at optimal and non-optimal values of process parameters [107, 120].

6.1 Validation of physics-based models. In the AM literature, experimental data has been used to validate individual physics models such as melt pool model and solidification model. Schwalbach et al. [92] validated a calibrated Discrete Source Model for melt pool prediction using single track experimental results. The prediction is tested against empirical observations of melt pool geometry produced by a multi-vector scan pattern. Gan et al. [121] validated the melt pool geometry by measuring the concentration of surface-active element sulfur using Auger electron spectroscopy (AES). Hu and Kovacevic [122] validated the thermal behavior of the molten pool using images collected from a coaxially installed infrared camera. Wang et al. [123] validated the prediction of differential thermal analysis using experimental data. Song et al. [124] validated the prediction of thermal gradient directions using grain growth orientations obtained from electron backscatter diffraction (ESBD) analysis. Rai et al. [125] validated a solidification model using experimental characterization of the microstructure and found that microstructure varies with location due to spatial variation of the cooling rate. Wang et al. [123] also validated the Scheil solidification diagrams using SEM images of the designed alloys.

AM process is simulated using a suite of multi-physics, multi-scale models. Considering an example of laser powder-bed fusion, the powder bed model can be simulated using the discrete element method. The output from the powder bed model such as packing density and powder bed porosity will be the input for the heat source model and subsequently the melt pool model [80]. Generally only the temperature data (the melt pool model output) is measured. In that case, it is not possible to validate individual models and the estimated error is the combined effect of three models. However, in the case of melt pool model output feeding into a residual stress model, both temperature data and deformation/residual stress data may be available for validation. In this case, the first model can be validated individually, but the measurement corresponding to the output of the second model combines the contributions of both physics, which makes it difficult to validate the second model individually. In that case, the validation result of the first model (i.e., discrepancy) needs to be propagated in a systematic way through the second model in order to achieve isolated validation of the second model. A further complication arises when there is two-way (feedback) coupling between two models; for example, the solidification is affected by temperature of the melt pool, however solidification affects the temperature, thus creating a two-way coupling.

Several studies have been reported w.r.t. the validation of multi-physics and multi-scale models in AM. For instance, Yang et al. [126] validated a process-structure model using published experimental data in the literature. Khomenko et al. [127] validated a coupled heat transfer and solidification kinetics model developed in the OpenFOAM framework using single track laser cladding experiments. The predicted macro and micro parameters of the track were compared with the actual parameters of the deposited track in their validation study [51]. Gu et al. [128] validated a multiscale numerical simulation model that considers complicated powder-laser interaction, heat and mass transfer behavior. Li et al. [129] combined FE models at microscale and macroscale to predict the mechanical properties of LPBF parts and compared them with experimental measurements. Tang et al. [130] validated their multi-scale modeling framework for the evaluation of structure-property relationships in AM parts with physical experiments. However, these studies compared the final output of the AM process, not the individual components; thus the validation was in an overall sense.

The above validation studies have not considered the various sources of uncertainties in the individual model during validation and instead validated the model for a nominal case or a few selected cases. Inclusion of UQ results in validation would make the models more useful for real-world decision-making [129]; such studies are reviewed a little later in this section. Some experimental studies do not report the measurement uncertainty in detail, but only provide nominal values. Even when the measurement uncertainty is reported, it is often in terms of summary statistics such as mean and standard deviation. Such limited information hampers rigorous validation under uncertainty, and may need the incorporation of additional statistical analysis techniques [131].

Several types of validation metrics and methods that assess the agreement between prediction and observation in the presence of uncertainty in both have been developed in the UQ literature. These include classical hypothesis testing, Bayesian hypothesis testing, probabilistic distance and area metrics, and information-theoretic divergence metrics [119]. In validation, it is valuable when possible to distinguish between the effects of aleatory and epistemic uncertainty sources on the validation assessment, in order to guide decisions regarding model refinement vs. additional testing [4]. The extension of these validation techniques to multi-physics, multi-scale AM process models needs to be investigated in future work. Further, validation methods for chained, hierarchical and coupled models have been explored in the UQ literature using the structural equation modeling approach [132, 133], but are yet to be extended to AM.

Currently model validation efforts mostly focus on scalar output QOIs, e.g., comparing the model prediction and experimental observation at only a few spatio-temporal locations [134]. As discussed earlier, the outputs of AM models and processes are varying over space and time (e.g., temperature profile, residual stress, porosity, delamination, geometrical accuracy and roughness). In AM parts, the material microstructure is also formed when the part is being manufactured. This highly dynamic process, typically under high-temperature conditions, leads to non-homogeneous and spatially correlated mechanical properties. Thus, it is necessary to validate the spatio-temporal outputs of the model to correctly evaluate the quality of the model. Ao et al. [135] extended the aforementioned probabilistic validation metrics to quantities varying over time. Three validation metrics were proposed to enable model validation in the time-domain: instantaneous reliability, first-passage reliability, and accumulated reliability. The extension of this approach to spatio-temporal validation of AM process models can be considered in future work.

Experimental data is needed in model validation. Proper allocation of experimental resources is necessary to perform validation of different models (e.g., how much data is enough for the melt-pool model validation or solidification model validation?). Similar to calibration, design of validation experiments to collect the most informative data for the validation of AM process models is necessary for efficient resource allocation. Several methods have been proposed in the literature for validation experimental design [135–137]. The extension of these methods to AM model validation can be investigated in future work.

One of the major bottlenecks in the validation of AM parts is the computational expense of running the sophisticated simulation models. Full-scale simulations are prohibitively expensive. For example, thermal and mechanical FE analyses of a planar spring (40 mm × 65 mm) manufactured using fused filament fabrication (FFF) took 300 minutes and 900 minutes respectively [138]. Moran et al. [139] used the principle of superposition part-scale thermal modeling for the PBF process to predict thermal fields. The simulation time for the V-22 osprey link of dimension 15.3 cm × 1.0 cm× 3.9 cm (maximum length scales) was reported as 18 hours. Additionally, the models have to be run multiple times to quantify the uncertainty in the prediction.

Nasab et al. [140] printed and conducted experiments on parts of dimension $20mm \times 20mm \times 20mm$ to study the effects of surface quality and volumetric defects on fatigue properties of AM parts. Parts of such volume cannot be directly simulated and intelligent modeling techniques need to be explored. Thus researchers have focused on developing models for a single-scan or part-scale models [141]. In rare cases where the entire part is considered, the dimension used is generally small in order to make the computation feasible [105, 107]. On the other hand, it may not possible to reliably print such small parts. Even if printing small parts is possible, the measurement of the QoI for such parts is challenging due to the errors in measurement being of the same order of magnitude as the QoI itself. Adaptive mesh refinement techniques along with access to high performance computing resources has been suggested to tackle this issue [141].

6.2 Validation of data-driven models. Given the computational challenges associated with physics-based modeling and the need for substantial understanding of the AM process to develop physics-based models, data-driven ML models of the AM processes are increasingly being pursued in recent years, as described in Section 2. Data-driven models can be validated using cross validation techniques such a k-fold validation. It is also important to select the optimal types and tuning parameters of the models (e.g., number of layers in a deep neural network), and avoid data overfitting. In the case of data-driven models, the available data is typically split into two categories – training data and testing data. The training data is further split for cross-validation purposes.

Since the raw material for some metal alloys are expensive, AM parts can be printed only in limited quantity. Physics-informed machine learning (PIML) models were discussed in Section 2, which leveraged physics knowledge or physics-based models to

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build models with a small number of experiments. The PIML models were validated using additional experimental data [73].

6.3 Measurements. Most of the experimental studies in AM have concentrated on temperature measurement using infrared cameras and high- speed cameras, since the temperature field directly impacts the microstructure and hence the material properties of the part. These measurements can be used to calibrate and validate the physics-based model. However, there are several challenges associated with these experiments, which call into question the accuracy of the model calibration and validation results. Flood and Liou [142] explored methodologies for the validation of thermal modeling and related attributes such as stress and microstructure. The modeling of the thermal history can be validated using direct or indirect measurements. In the direct method, the temperature is measured whereas in the indirect method a different quantity such as melt pool depth (linked to temperature) is measured to validate the thermal history. Where possible, direct measurement is preferable over indirect method. The most important data that needs to be collected is the melt pool temperature in the vicinity of the heat source but the laser obstructs the field of view. Since it is not possible to observe the scanning process from the top, the cameras are set up at an angle and this requires modifications to the AM printer [143].

Pyrometry-based measurement (non-contact measurement of temperature based on thermal radiation emission) relies on absorptivity, emissivity, reflectivity, and transmissivity properties of the material [144]. Since the properties are not accurately known or measured, the uncertainty in these values leads to inaccurate and unreliable measurement of the surface temperature [143]. The effects of vapor plume and their reflection, and the camera angle, also present difficulties in measurement and in some cases the observations cannot even be used, such as in the estimation of melt pool width [145]. High vapor flux in the melt pool causes material spatter, and variability in cooling rate results in an inhomogeneous product [146]. The measured signal has noise and is also impacted by the camera angle and reflection.

Uncertainty in measurement is also caused by data processing algorithms [147]. The choice of noise filtering techniques and corresponding filter parameters significantly affects the processed data, thus affecting the calibration and validation results. Also, large amount of data is collected in the form of images and videos during the monitoring process (e.g., with optical or thermal cameras). It is important to choose the most useful and optimal data in a systematic way. Given these issues, VVUQ studies have not yet been able to fully leverage the benefits of experiments.

AM machines tend to be expensive. Many researchers developing computational models do not have access to experiments and thus rely on experimental data found in the literature for model validation. The properties of raw materials and operating conditions significantly vary from one printer/laboratory to another, and all the information a modeler needs may not be reported. This is a considerable challenge for AM model validation activities. To address the challenges associated with the accuracy and sufficiency of measurement data for AM model calibration and validation, the National Institutes of Standards and Technology (NIST) has been publishing information on a series of controlled benchmark tests known as Additive Manufacturing Benchmark Test Series (AM-Bench) [148]. The main goal of AM-Bench is to provide rigorous, highly controlled AM benchmark test data using different measurement techniques and materials along with the relevant modeling information to allow modelers to evaluate the predictive accuracy of their simulation results.

7 Uncertainty aggregation

In the previous sections, the focus was on individual steps of uncertainty quantification such as model verification, calibration, and validation. Next, the results of these activities need to be integrated for the purpose of overall uncertainty quantification in the model prediction. Note that this is different from simple uncertainty propagation. Uncertainty propagation is simply the propagation of probability distributions (of aleatory inputs) through a (deterministic) model to compute the distribution of the model output. Epistemic uncertainty sources such as unknown model parameters and various types of model errors estimated during the verification, calibration, and validation steps do not propagate in a straightforward manner, and thus have to be aggregated systematically. The Bayesian approach to information fusion enables developing a rigorous framework to aggregate different types of uncertainty quantified in different steps. Such an aggregation approach was first proposed by Sankararaman and Mahadevan [83] and extended by Li and Mahadevan [149]. This approach was applied in Ref. [150] for the Bayesian calibration of material properties. Recently, Jiang et al. [151] extended the method to model discrepancy quantification and showed that the integration of V&V with Bayesian calibration has the potential to improve the accuracy of Bayesian calibration. The developed method has been applied to calibrate the melt pool geometry (length, depth, and width) using the AM-Bench experimental data [152].

Uncertainty aggregation in AM is an important research topic that needs to be investigated in the future, due to the presence of multiple models for different process physics and at different scales. The outcome of uncertainty aggregation across multiple physics and scales is uncertainty quantification in the prediction of output QOIs such as geometric accuracy, residual stress, porosity etc., all of which are quality indicators of the AM product. This uncertainty information can then be used in AM process optimization and control, as discussed in the next section.

8 AM process optimization and control under uncertainty

After the uncertainty in the AM product QOI has been quantified, the next step is decision-making under uncertainty. In the context of AM, two major decision-making tasks are process design and process control. Process design involves finding the optimal parameters for the AM process *before* the printing starts whereas process control refers to changing the process parameters in real-time *during* printing. Both process design and process control aim to improve the quality of AM product. A review on quality-related research in AM can be found in [153]. A recent article [154] explored the concept of six-sigma in quality management in AM and identified the need for decision-making under uncertainty in AM.

Some studies on the effect of AM process design parameters on the QoI focus on design on experiments (DoE)-based parametric studies with physical experiments. Khosrani et al. [155] used Taguchi DoE to print several parts with varying process parameters and studied their effects on QoI using multivariate analysis of variance. However, this approach does not have rigorous UQ. Two types of mathematical formulations can be considered for optimization under uncertainty: (a) *robust design optimization* (RDO) [156] where the mean and the variability of the objective function are optimized and the constraints are satisfied within bounds that account for uncertainty, and (b) *reliability-based design optimization* (RBDO) [157, 158] where optimization is performed to achieve a desired threshold of reliability. A few studies on AM process optimization under uncertainty have used these optimization formulations. Wang et al. [159] optimized preheating temperature, laser power, and scanning speed for an LPBF process with the objective of maximizing equiaxed grains in the microstructure. Kapusuzoglu et al. [105] optimized the process parameters such that the bond quality between extruded polymer filaments is maximized in FFF AM process. For an AM part to be of acceptable quality and be certified, multiple QoIs need to be optimized concurrently. Some of the objectives might be conflicting; thus, multi-objective optimization has also been explored in AM. Nath et al.[107] optimized process parameters such as extrusion temperature, extrusion velocity, and layer thickness with the

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objective of maximizing geometric accuracy and minimizing print time. Kapusuzoglu et al [120] considered multiple objectives of maximizing the mean geometric accuracy and bond length while minimizing the variance in geometric accuracy and bond length to design the process parameters.

Most multi-objective optimization studies assume independent responses and do not consider correlations between the multiple objectives. For example, low bond quality is correlated with low tensile strength in an AM part. Aljarrah et al. [160] proposed an approach for data-driven modeling and optimization with multiple correlated objectives. The two objectives considered – ultimate tensile strength and elapsed time – are scalar quantities. However, this study did not consider uncertainty. Presence of high-dimensional response, common in AM, further complicates the optimization of process parameters. Using techniques such as principal component analysis, SVD, etc. for dimension reduction and mapping the correlated outputs to an uncorrelated space can be explored to handle these challenges for AM.

As seen in Figure 2, the models representing the AM process may be *weakly (one-way / sequentially) coupled* or *strongly (two-way / fully)* coupled to each other. For example, consider the coupling between a finite element (FE) melt pool model and a cellular automaton (CA) solidification model to predict the microstructure of an AM part. In the weak coupled mode, the temperature history obtained from the melt pool model is used as an input to the solidification model to predict the microstructure; but no feedback from the solidification model to the melt pool is considered. In the strongly coupled mode, the fraction of solid increments are fed back to the FE model to update the temperature field after each time step [161]. Strongly coupled analysis is more accurate but computationally more expensive than weakly coupled analysis. When strongly coupled models are used, multidisciplinary analysis (MDA) approaches must be employed for uncertainty quantification [162, 163] and optimization. Martins and Lambe [164] reviewed and classified several multi-disciplinary design optimization (MDO) architectures. Several studies have investigated the Bayesian approach for MDO under uncertainty [165–167]. However, MDO approaches have not been implemented in AM research due to the high computational cost of incorporating strongly coupled AM models. Various optimization algorithms and methods are available in the literature that may be employed to aid AM process optimization. However, a general review of optimization techniques is outside the scope of this work. The discussion here is restricted to approaches for optimization under uncertainty.

Even starting the manufacturing process with optimal process parameters does not guarantee parts of good quality. It is necessary to take into account the possible anomalies in the print environment during manufacturing such as changes in the laser power [168] to print parts with consistent quality. This requires updating the information about the print environment during printing. This brings in the idea of a Digital Twin, which is a virtual representation of an individual physical system where data from the physical system is used to update the virtual representation over time [169]. As with other industries such as aerospace, cyber-physical systems, manufacturing systems, structural health monitoring, etc. [170], the introduction of digital twins for quality management and production efficiency management is quite natural in AM [171]. Studies have focused on digital twin for AM machines [172] and AM parts [173]. However, DT in AM is still in a very early stage and is yet to be demonstrated for real-time process control.

Research in AM process control has mostly focused on improving a few elements, such as AM process modeling and in-situ measurement. Other studies have focused on feedback control strategies using simplified simulation models [174–177] or direct observation data [178–180]. Reutzel and Nassar [181] surveyed sensing and control methods to improve metal-based AM process. Charalampous et al. [182] reviewed the various non-destructive testing methods for quality control in different AM processes prior, during, and after the manufacturing phase. Lhachemi et al. [183] reviewed the application of feedback, based on both traditional control techniques and augmented reality, in AM. All of these studies and methods are deterministic and do not incorporate any uncertainty quantification. Megahed et al. [168] proposed a framework for early stage identification of potential problems in the AM process. However, decision-making in the case of part quality deterioration is not discussed. The capability of a Bayesian methodology to include uncertainties and to update the state of the system makes it an obvious choice for AM process control. Nath and Mahadevan [111] presented a Bayesian layer-by-layer strategy of predictive quality control of an AM part. The model discrepancy term is updated at every layer using the real-time experimental data which incorporates information about anomaly in the printing environment, if any. The resulting process control approach allows the operator to make decisions about the manufacturing process based on real-time information: terminate, continue as is, or update process parameters for subsequent layers, thus saving material and energy.

Process control methods in AM are in early stages of development and implementation. There are several challenges for the implementation of AM process control algorithms. First, the models used in the algorithm need to be extremely fast and accurate. Second, the data acquisition from experiments and data processing has to be efficient for process optimization on the fly. Third, a related research area is the effect of dwell time in AM [184] in case the printing needs to be paused in order to update the process parameters. Finally, the control algorithms also need to be validated with experiments.

9 Opportunities and future needs

For the VVUQ of physics-based models, the following tasks have to be completed before the VVUQ process begins: (1) development of conceptual, mathematical and computational models for the physics phenomena being modeled; and (2) identification and design of appropriate experiments for the calibration and validation of the physics model prediction. Once these tasks are completed, the specific VVUQ tasks w.r.t. physics-based models involve:

(1) Code verification (i.e., verifying the software implementation of the physics model);
(2) Calculation verification (i.e., verifying the numerical solution for accuracy, convergence etc. in comparison to benchmark solutions);
(3) Calibration of physics model parameters (i.e., using experiments to estimate the values of model parameters) and
(4) Validation (i.e., comparison of simulation outcomes and experimental outcomes).

The main steps for VVUQ in data-driven models may be listed as:

(1) Gather and split the data (for training, cross-validation, and testing);
(2) Select the ML model type and implement the training algorithm;
(3) Verify the coding and calculation of the ML model using benchmark examples;
(4) Train, test (cross validate), and validate the ML model

However, several new developments are needed to accomplish VVUQ for AM. Since the physics-based AM models are multi-physics and multi-scale, some with high-dimensional outputs, appropriate calibration, verification and validation techniques need to be developed. The experiments for validation and data-driven modeling are challenged by the variability and measurability of relevant quantities, and by their high cost. Given these challenges, the following activities need to be undertaken in order to advance the state of the art in applying UQ to AM:

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(1) Develop protocols for reproducible AM experiments and identify appropriate data quality assessment techniques.
(2) Develop advanced solution verification methods for physics-based AM models (multi-physics and multi-scale).
(3) Develop new validation metrics and methods for coupled multi-physics models in AM.
(4) Extend model calibration techniques for high-dimensional response measurements (e.g., thermal camera images of temperature measurement).
(5) Develop new techniques for the aggregation of V&V and UQ results for individual models towards overall UQ of the AM process, in order to support certification and quality control efforts.
(6) Develop procedures to separate the contributions of aleatory and epistemic uncertainty sources to the V&V and UQ outcomes, in order to support decision-making and resource allocation for uncertainty reduction.
(7) Develop methods for sensitivity analysis that compare the relative contributions of multiple uncertainty sources in the presence of coupled and multi-scale models, physics-based and data-driven models, and experimental uncertainties.
(8) Develop use cases that demonstrate the implementation of the above activities by leveraging test results such as those published in AM-Bench [148].
(9) Develop standards for the above methods and procedures, including the V&V and UQ process flows, in order to facilitate industry acceptance of V&V and UQ techniques for AM.

10 Conclusion

The state of the art in the implementation of UQ approaches to additive manufacturing are surveyed in this paper. The research needs and possible paths towards implementation are also identified. In general, AM models consist of both physics-based and data-driven models, thus different VVUQ process flows need to be followed for each type of model. Future research and standardization activities need to develop methods and procedures to address the challenges presented by multi-physics, multi-scale models in AM with spatio-temporal outputs, complexity and quality of experimental measurements, and heterogeneous uncertainty sources.

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