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Uncertainty quantification in prediction of material properties during additive manufacturing

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ABSTRACT

Based on our experience gained from uncertainty quantification (UQ) of traditional manufacturing, this paper discusses UQ for additive manufacturing with a focus on the prediction of material properties. Applications of UQ methods in traditional manufacturing are briefly summarized first. Based on that, we investigate how the state of the art UQ techniques can be applied to AM process to quantify the uncertainty in the material properties due to various sources of uncertainty. The UQ of ultimate tensile strength of a structure obtained from laser sintering of nanoparticles is used as an example to illustrate the proposed UQ framework.

1. Introduction

Additive manufacturing has been successfully applied to the manufacturing of metal components with complicated geometries (e.g., engine rotor blades) [1]. It has a huge market potential of several billion dollars [2]. Current AM techniques for metal component manufacturing include stereolithography (SLA) [3], fused deposition modeling (FDM) [4], laminated object manufacturing (LOM) [5], selective laser sintering (SLS) [6], selective laser melting (SLM) [7], direct metal deposition (DMD) [8], laser metal deposition (LMD) [9], direct metal laser melting (DMLM) [10], and others. The most widely used ones are powder bed fusion-based AM processes (i.e., SLS, SLM, LMD, or DMLM), which are also the focus of this paper.

In the laser powder bed fusion process, the powders are delivered to the powder bed layer by layer and the powders are melted by the laser beam according to laser paths defined according to the 3D computer aided design (CAD) model. Due to various sources of uncertainty involved in the processes from powder bed forming to melting and solidification, variability is present in the properties of the manufactured metal components. As a result, it is hard to repeat the manufacturing of a high quality product and a trial-and-error approach needs to be employed to get a product with high quality. This becomes a major hurdle for the wide application of metal-based AM techniques. The fundamental reason for this limitation is that the variability in the manufacturing processes has not been properly captured.

A key to resolve the aforementioned problem is to use uncertainty quantification (UQ) techniques during the AM process. Despite the fact that UQ techniques have been studied for traditional manufacturing processes, their application in AM process is still at its early stage. Only a few examples have been reported in the literatures on UQ in AM [11–13]. In addition, currently reported UQ methods in AM are mainly based on experiments and are performed at the process level. This will result in excessive material wastage, increase product development cost, and delay the product development process [14]. A generic UQ framework built upon a good understanding of the fundamental principles of the AM process will significantly benefit the widespread use of the AM techniques. The understanding of the material properties resulting from additive manufacturing and the associated UQ is thus an important need in fully realizing the promise of AM.

This paper focuses on leveraging our experience in UQ of traditional manufacturing to UQ in the prediction of material properties during AM. Two examples of the UQ of traditional manufacturing process are presented first. Based on that, we discuss the challenges related to the UQ of the AM process. Solutions of these challenges will then be introduced through the employment of the state of the art UQ techniques. Finally, a laser sintering model of iron nanoparticles, which is an important example of a micro AM process, is used to illustrate the application of UQ techniques in AM of metal products.

The remainder of the paper is organized as follows. Section 2 provides a brief summary of our experience with UQ in traditional manufacturing. Section 3 discusses the UQ of material properties prediction in the AM process. A laser sintering example of nano-particles is given in Section 4 to demonstrate some of the discussed UQ techniques, and concluding remarks are given in Section 5.

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2. UQ in traditional manufacturing

Recent efforts in UQ of traditional manufacturing have been pursued along two interesting directions: (i) multi-scale modeling that links the manufacturing process parameters to the microstructure and to macro-scale properties, and (ii) macro-scale linkage of multiple manufacturing processes. The first direction is explained in details as below.

Cai and Mahadevan [15] used multi-scale modeling to investigate the effect of uncertainty in material initial condition and manufacturing process parameters on the microstructure. The uncertainty in the microstructure is then propagated to the uncertainty in the macro-level material properties as shown in Fig. 1.

As shown in Fig. 1 (a), a two-dimensional dual phase polycrystalline microstructure is simulated based on the initial condition of the grain cores (generated using stratified MCS) and the manufacturing environment. Then a homogenization method is applied to predict macro-level properties. The cooling schedule of the alloy is used to illustrate the methodology, and Young's modulus is the prediction quantity of interest. Even with a given cooling schedule, spatial variation of temperature affects the microstructure and properties as indicated in Fig. 1 (a); this variability is also incorporated through a random field representation of the temperature. Fig. 1 (b) shows the variability of Young's modulus obtained under different coefficients of variation of the temperature, which is presented as spatially varying random field (RF). It shows that the variation in the Young's modulus can be reduced significantly by reducing the uncertainty in the manufacturing process parameter (temperature). The UQ methodology uses a Kriging surrogate model [16] for computational efficiency, since a large number of runs of the multi-scale analysis are required corresponding to multiple realizations of the uncertain variables (i.e. uncertainty in the initial condition of the grain cores and temperature of manufacturing). The relative contributions of both aleatory and epistemic sources to the overall bulk property uncertainty are quantified using a global sensitivity analysis (GSA) approach (discussed in Section 3). The GSA method and surrogate modeling method is employed to identify the most important uncertainty sources and reduce the computational effort required during the UQ process. The sensitivity analysis also provides guidance for effective quality control of the manufacturing process in order to meet the desired uncertainty bounds in the bulk property estimates.

The above discussed research is about UQ of only one process model. Manufacturing of any product requires multiple processes and sub-processes, and UQ for such a network of processes is not straightforward. The uncertainty sources occur at different stages of the manufacturing process and do not combine in a straightforward manner; the combination could be linear, nonlinear, iterative, or nested. Nannapnaneni et al. [17] found a Bayesian Network (BN) approach to be advantageous in the uncertainty aggregation of such a complicated manufacturing network. The Bayesian network approach can also incorporate GSA and surrogate modeling techniques to reduce both the number of variables and the computational cost.

The above discussions briefly summarize successful applications of the UQ techniques to traditional manufacturing process. Next, we will discuss the UQ of material properties prediction during the AM process.

3. Uncertainty quantification during additive manufacturing

In this section, we first briefly introduce the models in the AM process. Following that, we will discuss the UQ of AM process.

3.1. AM process models

During the AM process, the models used to predict the process performance can be roughly classified into five models as shown in Fig. 2. The outputs of the heat source model and powder bed model will act as inputs of the melting pool model. The output of the melting model will be used as input of the solidification model to study the evolution of the microstructure during the AM process. The solidification model and the melting pool model will provide information for the residual stress analysis model and other macro-level analysis models [18]. The analysis and simulation methods used in each model are also given in Fig. 2. Since there are connections between different simulation models, the uncertainty at lower levels such as that in the powder bed model will propagate to the uncertainty in the solidification model, which will then be presented in the residual stress model. This brings more challenges to the UQ of AM process than in traditional manufacturing.

In the subsequent sections, we will first identify various sources of uncertainty in the AM process and then discuss the challenges in UQ of AM and provide potential solutions.

3.2. Identification of uncertainty sources

Similar to the UQ of traditional manufacturing, the uncertainty sources in the AM process can be classified into two categories: *aleatory uncertainty* and *epistemic uncertainty* [19]. Aleatory uncertainty refers to natural variability, which is irreducible. Epistemic uncertainty refers to the uncertainty due to lack of knowledge regarding model inputs and

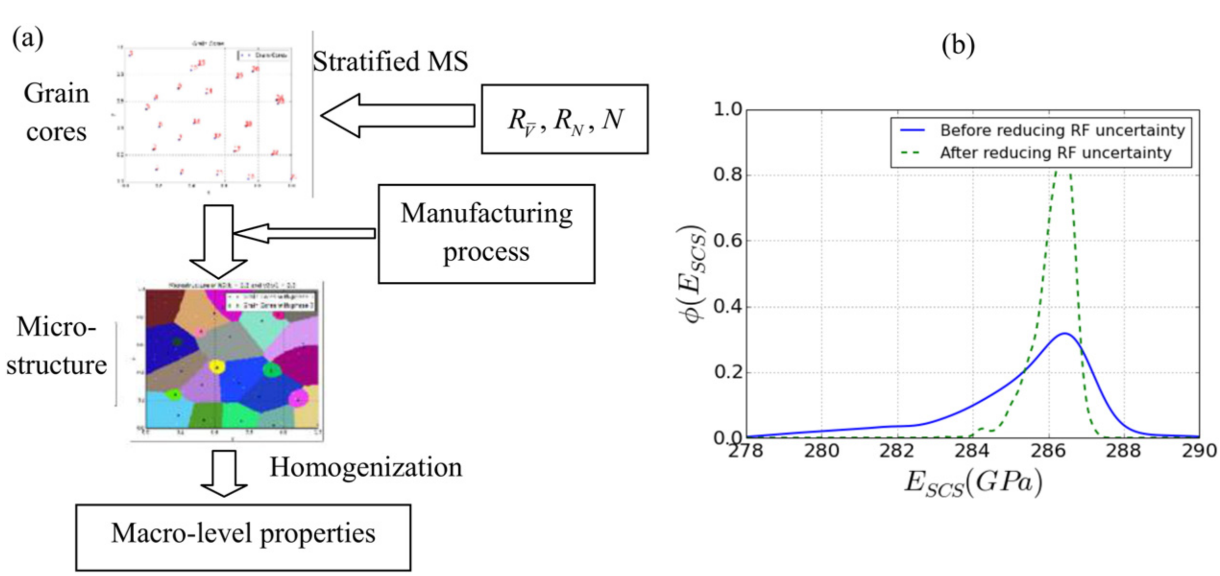

Fig. 1. UQ of Young's modulus for two-phase polycrystalline alloy [15].

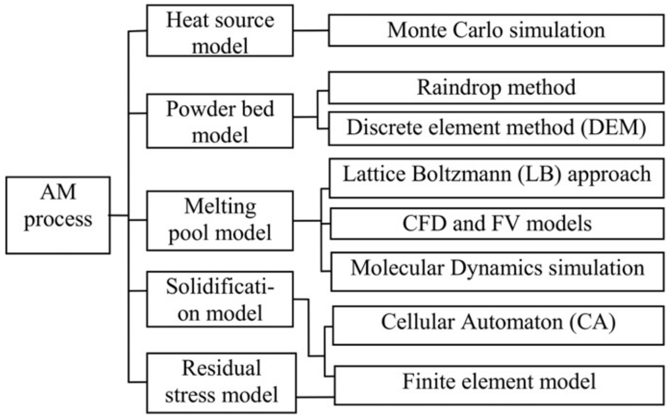

Fig. 2. Models of AM process.

parameters and the approximations and assumptions introduced during the modeling process. Epistemic uncertainty can be reduced by collecting more information or by more refined modeling. Both aleatory and epistemic uncertainty sources are involved in the five AM process models mentioned in Section 3.1, as summarized below.

3.2.1. Aleatory uncertainty

There are numerous sources of aleatory uncertainty. We only list several examples here. Some of the aleatory uncertainty sources include natural variability in the radius of the powder particles, fluctuation of laser scan speed, variation of mechanical properties (elasticity, friction coefficient, and damping coefficients) of powder particles, variation of diffusion coefficient of the material, uncertainty of absorption coefficient, variation in the temperature boundary condition, and measurement errors.

3.2.2. Epistemic uncertainty

As shown in Fig. 3, epistemic uncertainty can be further divided into two groups, namely *data uncertainty* and *model uncertainty* [20]. Data uncertainty may come from limited data or imprecise measurements. In addition, even if some quantity is deterministic, we may not be able to directly measure it but only infer from observations of other variables (inputs and outputs). In that situation, there is also epistemic uncertainty in the modeling of the AM process parameter (model coefficients). For instance, we may only have limited information about the drag coefficient of the powder particles during the melt pool modeling; the isolated manner of studying the blown powder process parameters may introduce epistemic uncertainty to the correlation coefficients between different parameters.

In addition to data uncertainty, the other important source of epistemic uncertainty is model uncertainty (difference between simulations and experiments). The model uncertainty comes from not only the assumptions, simplifications, and numerical discretizations made in various models, but also different methods (e.g. Eulerian or Lagrangian framework) of representing the problems. Examples include the use of discrete element method or rain drop method in the powder bed model, the simplification of the lattice Boltzmann (LB) approach in the melting pool model, and use of finite element or finite difference models to solve the partial differential equations (such as the blown powder model given in Ref. [18]) using numerical discretization. The assumptions and simplifications (such as spherical shape assumption of the powder particle and simplification of evaporation and Marangoni forces) result in model form errors. The numerical discretization introduces approximation errors to the model prediction. In addition, the computer simulation models are usually computationally expensive, and UQ techniques require multiple runs of the simulation models. For instance, a 3D LB method for the melting pool simulation is expected to take hours or even days. Therefore surrogate models are widely used as substitutes for the expensive simulation models while implementing UQ techniques. When surrogate models are used, they introduce additional approximation and uncertainty in the prediction, and need to be included in UQ. Note that the model coefficients such as coefficient of the material, friction coefficient, absorption coefficient are sources of epistemic uncertainty for a single instantiation of the process. These coefficients also have aleatory variability when multiple instantiations are considered (variation from product to product).

Next, we will investigate the challenges and corresponding solution approaches for UQ of AM process based on the above identified uncertainty sources.

3.3. Challenges and solutions in UQ of AM process

3.3.1. Challenges in UQ of AM process

The challenges in UQ of AM process arise mainly from two factors, namely *complicated nature of the problem* and *limited resources for UQ*. For each challenge, there are several research issues that need to be addressed. These two main challenges are discussed below.

3.3.1.1. Complicated nature of the problem. As discussed in Section 3.2, various sources of uncertainty are involved in AM. The first research

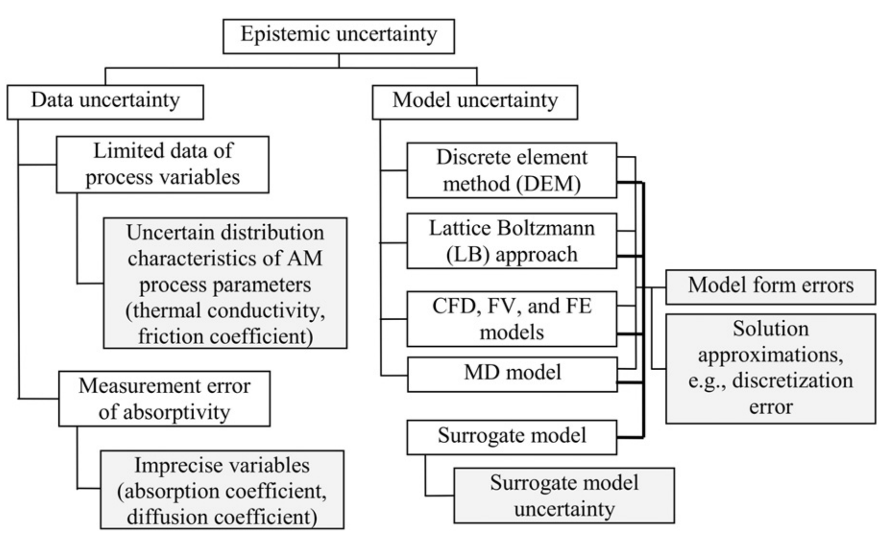

Fig. 3. Types of epistemic uncertainty sources in AM process.

issue that needs to be addressed in UQ of AM is how to effectively model these sources of uncertainty. After the modeling of the heterogeneous sources of uncertainty, how to effectively incorporate them towards the UQ of the quantities of interest needs to be studied.

Based on the modeling of uncertainty sources, UQ of AM is not straightforward. There are complicated connections between different simulation models and these models are present in a hierarchical manner. The simulation models cover multiple length scales, from micro-level to macro-level. Effective multilevel UQ methods are required for this kind of multi-level and multi-scale UQ problem.

There are also feedback couplings between different simulation models, such as the coupling between computational fluid dynamics model and finite element simulation model for the melting pool modeling and the coupling between finite element model and cellular automaton model for the microstructure modeling during solidification. Multidisciplinary UQ methods need to be developed for this type of problem. How to decouple the coupled simulations to efficiently perform UQ is also a research challenge.

In addition to the above research issues, another important concern is how to effectively account for the noise in the simulation model output and experimental observations. For example, we may get different simulation results for the same simulation model when the simulations are implemented by different researchers, even if the input settings are the same.

3.3.1.2. Limited resources for UQ. If we have unlimited computational resources, the UQ of AM process can be performed directly using Monte Carlo simulation (MCS). The challenge of limited resources for UQ can be attributed to three reasons: (1) large number of variables, (2) limited computational resources, and (3) limited experimental resources.

3.3.1.2.1. Large number of variables. As shown in Fig. 2, there are several models involved in each stage of the AM process, each model consists of numerous variables. This makes the UQ during AM process a high-dimensional problem. The large number of variables brings several difficulties. The first difficulty is that the computational demand for UQ will increase exponentially with the number of random variables. The second difficulty is that the output quantities of interest may be highly nonlinear in terms of these random variables. Accurately capturing the high-dimensional domain is very challenge. This high-dimensional problem also leads to the following two research issues.

3.3.1.2.2. Limited computational resources. Computer simulations are used to simulate each stage of the AM process, such as melting and solidification. These simulation models however are computationally demanding. During the process of UQ (e.g., Monte Carlo simulation), the simulation models need to be executed a large number of times. This has a high requirement on the computational resources. A research issue is how to effectively perform UQ of the AM process given the limited computational resources, such as how to reduce the number of training points required in the surrogate modeling. Besides, the limited computational resources may also degrade the accuracy of UQ. Balancing efficiency and accuracy of UQ within the constraints of computational resources is a major research issue for UQ in AM.

3.3.1.2.3. Limited experimental resources. Experiments are used in AM process to collect useful information and thus reduce the uncertainty in certain critical variables, by facilitating model calibration and model validation. Similar to the problem of computational models, we also have limited experimental resources. Arbitrarily performing experiments will result in significant wastage of materials, time, and cost. Given the limited experimental resources, how to efficiently collect the most useful information is a significant research issue.

Computer simulation models are often used to substitute experiments to reduce the time and cost of experiments. However, some simulations models may be more expensive than the experiments. Given the fact that both experiments and computer simulation models are expensive, how to effectively allocate resources for both simulations and experiments for effective UQ is worth pursuing in future efforts of UQ in AM.

Next, we will present solution approaches to the aforementioned challenges, based on state-of-the-art UQ techniques.

3.3.2. Solution approaches

3.3.2.1. Modeling of uncertainty sources. The aleatory uncertainty can be modeled as random variables for time-independent quantities, stochastic processes for time-varying quantities, and stochastic fields for space-varying quantities. For the modeling of epistemic uncertainty, the lack of knowledge regarding unknown quantities can be modeled using a Bayesian approach that systematically fuses available information and quantifies the reduction in uncertainty as more information becomes available. Interval variables and evidence theory can also be employed to model variables with higher uncertainty.

For the modeling of model uncertainty, the discrepancy between model prediction and experimental observation can be quantified using Bayesian calibration [21]; and Richardson extrapolation method can be used to model the numerical discretization error. A detailed description of various methods for quantifying the uncertainty sources can be found in Ref. [20].

3.3.2.2. Multilevel UQ and uncertainty aggregation. For the multilevel UQ and incorporation of heterogeneous sources of uncertainty, a BN [22] technique can be used. BN expresses the multivariate joint probability density function as a product of marginal and conditional probability density functions. Its capabilities in information fusion and incorporating heterogeneous sources of uncertainty have been demonstrated in various UQ application problems. At each level of the UQ problem, surrogate models can be built to substitute the individual (expensive) simulation models. The inputs and outputs of the surrogate models at different levels can then become nodes of the BNs and are connected together through the BN in a multi-level manner. In the case that we are not sure about the connection between different nodes, the connections between these kinds of nodes can be learned through Bayesian network learning techniques [23].

To address the challenge of coupling between different simulation models in UQ of the AM process, a recently developed likelihood-based approach for multidisciplinary analysis (LAMDA) [24] can be employed to efficiently decouple different models without sacrificing accuracy. After the decoupling of different models, the models can be integrated naturally using the BN technique.

3.3.2.3. Global sensitivity analysis (GSA). GSA quantifies the contribution of each input variable (X) to the variance of a quantity of interest (Y). This can play an important role in addressing the challenge of high-dimensional problems. The first-order Sobol' index measures the individual contribution of each variable without considering its interactions with other variables, and is given by [25]

$$S_i^I = \frac{Var_{X_i}(E_{X\sim i}(Y|X_i))}{Var(Y)} \tag{1}$$

where X_i is the i-th input variable, $X_{\sim i}$ is the vector of variables excluding variable X_i, $Var(Y)$ is the variance of Y, and $E_{X\sim i}(Y|X_i)$ is the expectation by freezing X_i.

The total effects Sobol' index measures the contribution of each variable including its interactions with other variables, and is given by

$$S_i^T = 1 - \frac{E_{X_{\sim i}}\left(Var_{X_i}(Y|X_{\sim i})\right)}{Var(Y)} \tag{2}$$

Recently an advanced method using an auxiliary variable approach has been developed to include both epistemic and aleatory uncertainty sources in GSA. Based on GSA, we can ignore the uncertainty sources with low contributions to the variance of the response variable and thus reduce the dimension of the problem.

3.3.2.4. Surrogate modeling. An important issue in surrogate model construction is the selection of training runs (i.e., runs of the original expensive simulation model). We have developed adaptive approaches such as efficient global reliability analysis (EGRA) [16] and global sensitivity analysis-enhanced surrogate (GSAS) [26] approaches in order to maximize the collection of useful information from the training runs and to overcome the challenge of limited computational resources.

3.3.2.5. Experimental design for model calibration and validation. In order to overcome the challenge of limited experimental resources, effective methodologies are required for optimal design of the experiments (i.e., selection of input settings) to maximize the information gain from the experiments. Experimental design can be conducted from a model calibration perspective, model validation perspective, or both. We have developed not only effective experimental design methods for calibration and validation, but also for identifying the optimal locations for sensors to collect data [27–29]. These techniques can be explored to solve the challenge of limited experimental resources for UQ in AM.

3.3.2.6. Resource allocation. Resource allocation provides information on what simulations to perform and what experiments to conduct. With regard to simulations, optimization techniques could be employed to identify when a high-fidelity simulation is needed, and when low-fidelity simulations are adequate, thus trading off between accuracy and efficiency [30]. With regard to testing, optimization techniques could be employed to decide how many experiments of each type need to be performed to maximize the uncertainty reduction from the data collection effort [31,32]. Resource allocation under uncertainty is one of most important techniques for solving the issue of limited resources.

3.3.2.7. Integration of calibration, validation, and uncertainty prediction. In the UQ of AM process, model calibration, validation, and forward uncertainty prediction are needed. Different techniques have different motivations. Integration of the results of calibration, validation, and uncertainty prediction can enhance our confidence in the UQ of AM process. To achieve the purpose of integration of calibration, validation, and uncertainty prediction, we recently developed a roll-up method [33], which can effectively taking advantage of currently available resources for the purposed of UQ. As shown in Fig. 4, the roll-up method can effectively incorporate the uncertainty in the model form quantified from model validation into the model calibration result.

Through the pursuing of the abovementioned UQ techniques, the challenges in the UQ of material properties prediction during AM process can be addressed in the near future. In the next section, the application of some of the above mentioned techniques will be illustrated using an example.

4. Example: UQ of selective laser sintering of nanoparticles

In this section, selective laser sintering (SLS) of Fe-Fe nanoparticles is used to illustrate the application of the UQ techniques in the AM process. Laser sintering of nanoparticles is one of main stages in the micro additive manufacturing (Micro-AM) process. The nanoparticles are first melted under a constant heating rate and cooled down under a constant cooling rate. After that, tensile test is performed on the structure to investigate the material properties after melting and cooling. In this example, the nanoparticles are assumed to be spherical. The radii of different particles are different due to natural variability and there may be a gap (i.e. d) between the two nanoparticles. Simulations of the laser sintering and tensile test of nanoparticles are performed using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [34].

4.1. Identification of uncertainty sources

To quantify the uncertainty in the simulation result, we first identify the uncertainty sources (i.e. Section 3.2). The aleatory uncertainty sources include the variability of particle radii, sintering temperature, and the gap between the particles due to packing of the powder bed. Since the LAMMPS model is used to simulate the process of sintering and tensile test, the epistemic uncertainty mainly comes from the simulation model. In the LAMMPS simulation, the Fe Embedded Atom Model (EAM) potential is used to approximate the energy between atoms. Since EAM is a regression model based on experimental data, there is epistemic uncertainty regarding the coefficients of the EAM potentials due to experimental variability and limited experiment data. Along with the epistemic uncertainty in the EAM potential coefficients, there is also uncertainty in the LAMMPS simulation result due to the simplifications and assumptions made in the molecular dynamics simulations. In this example, for the sake of illustration, the aleatory uncertainty in the geometry and sintering temperature, and the epistemic uncertainty in the EAM potential are considered.

4.2. Uncertainty quantification

Since LAMMPS simulation is usually computationally expensive for large scale problems, this results in the limited computational resource

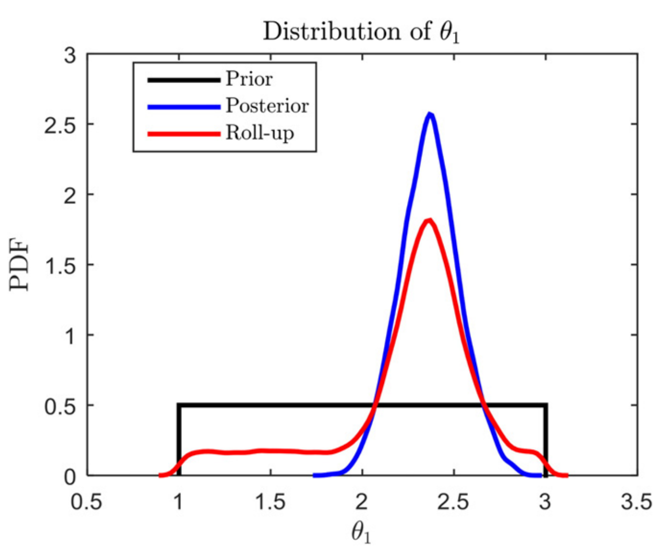

Fig. 4. Illustration example of roll-up method.

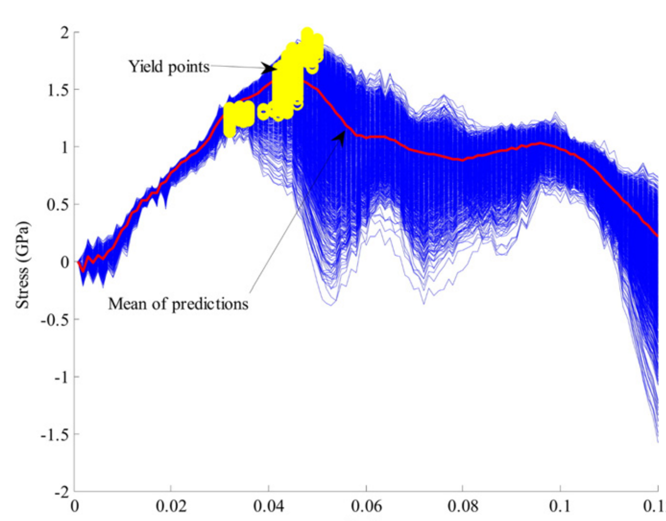

Fig. 5. Uncertainty quantification of the strain-stress curve.

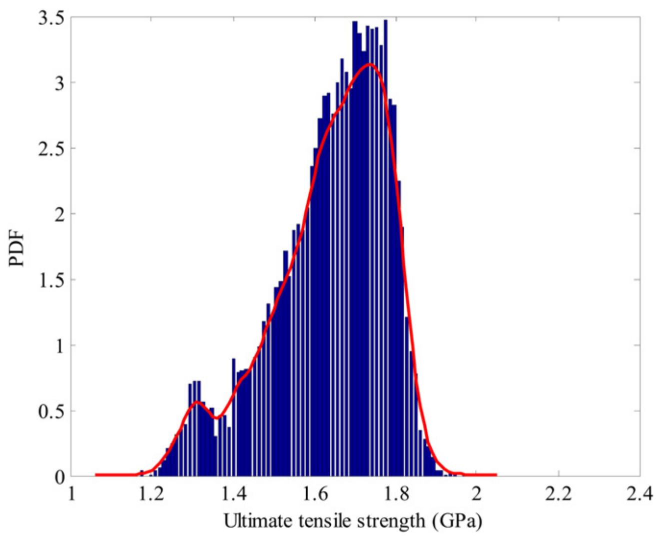

Fig. 6. Uncertainty quantification of the ultimate tensile strength.

issue as discussed in Section3.3.1. To overcome this challenge, the *surrogate modeling* method introduced in Section 3.3.2 is used. After the uncertainty sources are identified, training points of random variables are generated using design of experiments methods. Based on the LAMMPS simulations at the training points, surrogate models are built for the stress responses using the Kriging surrogate model method [16]. Since the surrogate models are computationally inexpensive, we directly perform MCS on the surrogate model to investigate the uncertainty in the strain-stress curves.

Fig. 5 shows 1000 realizations of the strain-stress curves obtained from MCS using the surrogate model by considering the above identified uncertainty sources. The mean prediction of the strain-stress curve and the ultimate yield points are also shown in the figure. By analyzing the uncertainty in the ultimate yield points, we obtain the uncertainty in the ultimate tensile strength. Fig. 6 gives the histogram of the tensile strength obtained from MCS and the fitted probability density function curve.

We also performed global sensitivity analysis using the GSA method discussed in Section 3.3.2 for this example to investigate the contributions of each random variable on the variability of the ultimate tensile strength. It was found that the uncertainty in the ultimate tensile strength of this numerical example mainly came from the epistemic uncertainty in the EAM potential. If we exclude the epistemic uncertainty of EAM potential, then the variability of sintering temperature is found to affect the variability of ultimate tensile strength more significantly than the other variables. Fig. 7 gives a flow chart of the UQ of laser sintering example.

5. Conclusion

Uncertainty quantification of the AM process plays an important role in achieving effective quality control of the AM process and thus realizing the significant market potential of the AM techniques in manufacturing metal components. Current application of UQ techniques in the AM process, however, is still in the early stages. This paper discusses how to leverage our experience in UQ of traditional manufacturing processes to implement the UQ of material properties prediction during AM process. The uncertainty sources and challenges in the UQ of AM process are identified first. Based on this, we discuss how to address these challenges through the state of the art UQ techniques. These discussions identify promising directions for the future research in the UQ of AM process. The example of UQ of laser sintering of nanoparticles provides an illustration on how to apply the UQ methods to AM.

Future needs include developing more rigorous AM process models to reduce the epistemic uncertainty, investigating the state of the art UQ methods to other AM models, and developing new UQ methods to address the multi-scale and multi-model coupling challenges.

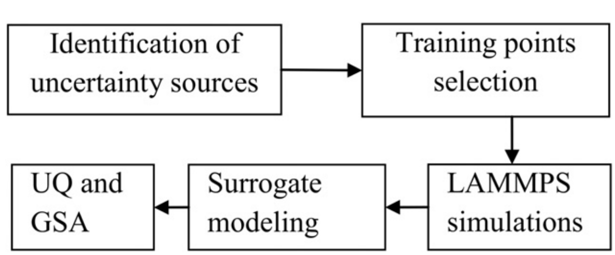

Fig. 7. Flowchart of UQ of laser sintering of nanoparticles.

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