Towards developing multiscale-multiphysics models and their surrogates for digital twins of metal additive manufacturing

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ABSTRACT

Artificial intelligence (AI) embedded within digital models of manufacturing processes can be used to improve process productivity and product quality significantly. The application of such advanced capabilities particularly to highly digitalized processes such as metal additive manufacturing (AM) is likely to make those processes commercially more attractive. AI capabilities will reside within Digital Twins (DTs) which are living virtual replicas of the physical processes. DTs will be empowered to operate autonomously in a diagnostic control capacity to supervise processes and can be interrogated by the practitioner to inform the optimal processing route for any given product. The utility of the information gained from the DTs would depend on the quality of the digital models and, more importantly, their faster-solving surrogates which dwell within DTs for consultation during rapid decision-making. In this article, we point out the exceptional value of DTs in AM and focus on the need to create high-fidelity multiscale-multiphysics models for AM processes to feed the AI capabilities. We identify technical hurdles for their development, including those arising from the multiscale and multiphysics characteristics of the models, the difficulties in linking models of the subprocesses across scales and physics, and the scarcity of experimental data. We discuss the need for creating surrogate models using machine learning approaches for real-time problem-solving. We further identify non-technical barriers, such as the need for standardization and difficulties in collaborating across different types of institutions. We offer potential solutions for all these challenges, after reflecting on and researching discussions held at an international symposium on the subject in 2019. We argue that a collaborative approach can not only help accelerate their development compared with disparate efforts, but also enhance the quality of the models by allowing modular development and linkages that account for interactions between the various sub-processes in AM. A high-level roadmap is suggested for starting such a collaboration.

1. Introduction

While the industrial revolution transformed manufacturing by introducing machines, further productivity gains were achieved by adding electrification and automation. It is now well accepted that additional increases in efficiency can be generated by incorporating artificial intelligence (AI) into machines [1] so that they "think for themselves," i.e., learn from historical data to perform a required task in the optimum possible way. A highly digitalized process, such as metal additive manufacturing (AM), lends itself well to this approach. The application of AI to AM through Digital Twins (DTs) will lower costs by reducing or eliminating waste and reducing human intervention, besides creating more reliable and efficient builds. Also, by assuring quality in the product, the DT will make AM a method of choice for producing

mission-critical components.

Since its inception more than two decades ago, AM has remained a high-end niche process. As a result, this enabling technology is yet to find widespread deployment in the commercial sector. There are several complex reasons for this, but chief amongst them are (1) poor process repeatability, which makes it challenging to build parts with quality assurance, leading to implications for certification, (2) expensive waste, attributed to the mostly trial-and-error nature of finding optimum process parameters, and (3) the high cost of characterization and inspection of components which limits the number of data sets required to develop a thorough understanding. However, AI can significantly improve the repeatability of the process, accelerating parameter development, and reduce waste, making it more attractive to manufacturers. Real-time closed-loop control supervised by AI can control the AM process within recommended process bounds. The same AI can find the optimum processing specifications for a given part before its build begins, as it contains process insights. The AI resides in a continuously updated virtual replica of the process called the DT, which controls the AM machine. It can supervise to keep the process on the optimal processing route or initiate changes to the process parameters in real-time to recover from an unexpected excursion. Thereby it assures quality in the process and, by extension, also in the product. The DT makes use of readily interrogatable AI that dwells in machine-learning (ML) models. ML models are derived from more detailed physics-based and/or statistics-based models of the process and experimental and/or field data. To develop reliable AI, usually sizeable amounts of high-quality data must be available. Since AM processes are slow and the builds expensive, relying solely on experiments or field data alone is likely to make the process of developing models slower and more expensive compared with complementing such data with those obtained from mechanistic models. Computational models can address this issue by taking a handful of physical data points as validation and multiplying these to create the 'big data' required for the ML models.

DTs are expected to guide smart factories of the Industry 4.0 era towards achieving previously unattainable levels of process productivity and part quality [2]. There is presently no consensus definition in the literature for the DT. However, for our purposes, we can define [2–9] the DT as an autonomous, dynamic, real-time virtual replica of an item (e.g., product, system, asset, city), service, or process in the physical domain. Its autonomous capabilities stem from the artificial intelligence (AI) embedded in the DT. Also, the word 'dynamic' in the definition alludes to the fact that it is a living representation, evolving with the updates and improvements that are gradually added to it. Importantly, the DT is not an isolated digital copy; instead, it maintains two-way communication with its physical twin. It receives real-time data from the sensors monitoring the physical twin and, in turn, provides real-time diagnostic control commands to the physical twin (Fig. 1). In an AM process, real-time temperature measurements are often a good indicator of how the process is progressing and can be used to modify process parameters

if and when required (see Section 3.1 later for a case study). The DT uses real-time data from its physical twin and other sources to enable learning, reasoning, and dynamic recalibration. The improved insight so obtained facilitates robust decision-making for optimizing the performance of its physical twin or keeping its execution within chosen limits by instantly recognizing anomalies. Several potential benefits accruing to a business from the deployment of DTs have been discussed in detail by others (e.g., [2,6,7,10–12]).

Although, as noted above, there are different types of DTs depending on the type of physical twins [4,13], we will consider only the process twin here since our focus is on the metal AM process. While the article will use the laser powder-bed fusion (LPBF) system as an example, most of the concepts discussed will be applicable across other metal AM systems, including direct energy deposition. For manufacturing process applications, including AM, the value of DTs is twofold. Not only can they be used as 'superhuman supervisors' that can 'see' a process in progress via multiple indicators and – if necessary – take real-time decisions to correct that process. They can also, using AI, help select optimum processing parameters a priori. This is because the AI is contained in the virtual models of the AM process, and these models can be run and queried even before the actual physical build of a part commences.

Recently published articles [6,11] indicate that, although maturing rapidly as a concept, the process DT is yet to find widespread deployment in factories despite some industrial giants such as General Electric, Siemens, PTC, Dassault Systems, and Tesla already reaping benefits from its use [14,15]. A recent review suggests that the situation is worse in the area of AM [16]. There are several reasons for this, including the current cost barrier as well as the fact that relevant skillsets in the AI and machine learning (ML) fields are not yet freely available.

The situation is changing rapidly, however. For example, in the area of metal AM, niche manufacturers such as Aconity3D [17,18] and Markforged [19] are making machines that run on open-source software that can be coded to set up the type of cyber-physical feedback and control loops characteristic of DTs. Therefore, efforts similar to that sponsored by *America Makes* and led by GE Global Research Center's (GEGRC) Additive Manufacturing Laboratory [20] can develop open-source software solutions. Such machines can currently take near-real-time physical action based on the process state as visualized by data from embedded sensors. They also accommodate the logging of data relating to numerous process parameters for the creation of big data meant for the training of ML models. Further, online sensor hardware needed for real-time data-logging has grown immensely in sophistication [21–23], and there are continuing efforts to extend its boundaries [24,25] – including through the use of open-source software solutions [26]. Software that facilitates the efficient sharing of information between components of a DT and its physical counterpart has also emerged and is already being used by some businesses [27,28]. Further, the science of big data has seen significant advances in recent times [29,30] and can increasingly support multidisciplinary data as well as progressively more complex ML. With the maturation of hardware, software, data analytics, and ML/AI over the coming years and their increased affordability, the stage will be set for the adoption of DTs in the AM industry. In a sign that engineers are preparing for such a future, the *American Society for Mechanical Engineers* (ASME) has formed a new Committee on Advanced Monitoring, Diagnostic, and Prognostic Technologies for Manufacturing [31].

Therefore, the time is now ripe for computational modelers to seize the initiative to build on the largely disparate multiscale modeling efforts in AM (e.g. [32–37]). A coordinated and well-funded global effort can result in the development of comprehensive and well-linked high-fidelity physics-rich software models which will provide high-quality process intelligence to metal AM DTs. In this article, we offer our collective thoughts on the subject to stimulate dialog across the AM community. Many of the opinions are based on a brainstorming session held a workshop attended by delegates from industry, academia, national laboratories, and government bodies, at an international symposium
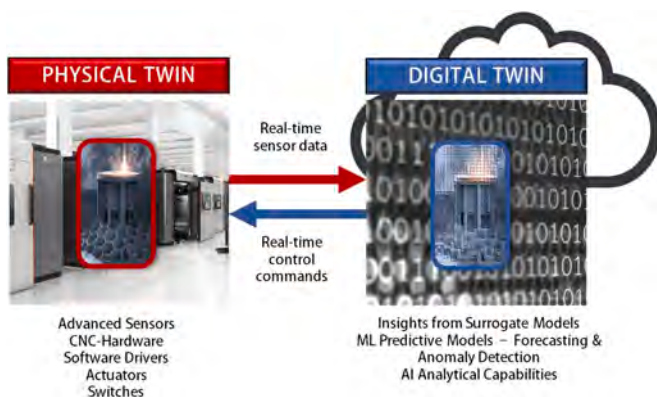

Fig. 1. Operation of a process DT in a real-time diagnostic control capacity.

organized by CSIRO in July 2019 in Melbourne, Australia, and thus have a broad, global perspective.

2. Role of physics-rich models within the DT ecosystem & in AM

A DT is developed by observing, quantifying, and, as far as possible, reproducing its physical twin's behavior. Different enabling technologies that come under the umbrella of Industry 4.0 contribute to the creation of the DT of a physical process [11].

2.1. The DT environment

An example of the ecosystem of a process DT is provided in Fig. 2. The physics-agnostic 'black-box' statistical relationships obtained from data sourced in the physical world as well as 'white-box' physics-derived relationships acquired from software models combine to produce the 'gray-box' data set. This data set is then used to create reduced-order models and physics-agnostic surrogate models, which are trained using ML methods. The surrogate models are simpler versions that mimic the mechanisms of the complex models, and so can be solved faster (i.e., in hours/days relevant to build times rather than weeks/ months). Physics models can use a limited number of data points taken from the physical world as validation. The models can then simulate the process's behavior in numerous additional scenarios, thereby multiplying the number of data points available for the training data set. This produces what is referred to as 'synthetic data', or 'capta'. A data set that is significantly expanded in this way can potentially result in higher fidelity surrogate models with robust predictive capabilities. In turn, these models can provide superior quality guidance to the DT.

The process models used by DTs are continually updated using data sourced from the physical twin via sensors. This allows the DT to accurately reflect the real-time state of its physical twin at any given moment. By continually learning from the physical twin, the DT increasingly encapsulates, over time, a more accurate version of its physical counterpart (mainly through reinforcement learning).

A crucial step in developing a DT is the creation of surrogate models that hold the process intelligence in a readily interrogatable form and are, thus, equipped for forecasting and anomaly detection. Once built, the DT can then consult these models in real-time for swift decision-making. As an example, if an instance of a physical process deviates from its desired path for any reason, the forecasting models can assist the DT to chart a path to recovery.

2.2. Extraordinary value of AM computational models

AM is a process that stands to gain tremendously from the application of computational modeling. There are at least two important reasons for this. Firstly, the process is inherently slow; this and the cost of raw material (powder) and subsequent material inspection mean each build is expensive. Consequently, the amount of experimental data that can be generated is limited, and so should be complemented with reliable data from computational modeling. Secondly, the AM process is challenging to observe in real-time, with many aspects of the process difficult or impossible to monitor (e.g., internal temperatures, stress state, etc.). High-fidelity simulations can reconstruct the process and at least partially address this obstacle.

Difficulties in obtaining measurements at the microscopic length scales, which are characteristic of nascent melt pools in AM, combined with the rapid nature of the ensuing solidification process, make it hard to observe and study the process purely through experimental methods. It can also be challenging to monitor the supporting sub-processes, e.g., powder coating or raking, that may affect part quality. Validated simulations can fill this gap by allowing us to 'see' the reconstructed processes conveniently, e.g., by freezing frames, and in the context of the underlying physics. Simulations are, therefore, an invaluable teaching tool – both for human operators and for DTs. They can show, for instance, the velocity distribution of powder particles during spreading as a function of parameters such as powder size and aspect ratio [38]. They can predict subsurface temperatures in an AM build and the developing stresses [9]. Physics-based models also aid in the faster discovery of optimal process parameters by screening out unsuitable material candidates and/or process parameter candidates efficiently, leaving only those that warrant further investigation through physical experiments. Further, computational models can predict dimensional inaccuracies that can occur, providing an opportunity to adjust process parameters before the start of a build [39,40].

Physics-based simulation is a powerful tool to understand the science involved in highly dynamic processes like AM, which are hard to observe physically. If the process route can be faithfully reconstructed based on available sensor data coupled with final, quantifiable outcomes like microstructure, defects, part distortion, and residual stresses, the process's digital replica may be used to obtain histories of various quantities at numerous locations of 'virtual probes.' We can have as many probes as we wish, and the simulation can be paused at different time points and the results interrogated to understand the link between cause and effect. In work published recently [41], researchers used high-fidelity simulations, coupled with synchrotron experiments, to capture fast, transient dynamics at the meso- and nanosecond scale. They discovered new spatter-induced defect formation mechanisms that depended on the scan strategy and competition between laser shadowing and expulsion. With the assistance of computational modeling, they were then able to derive criteria for stabilizing the melt pool dynamics and minimizing defects.
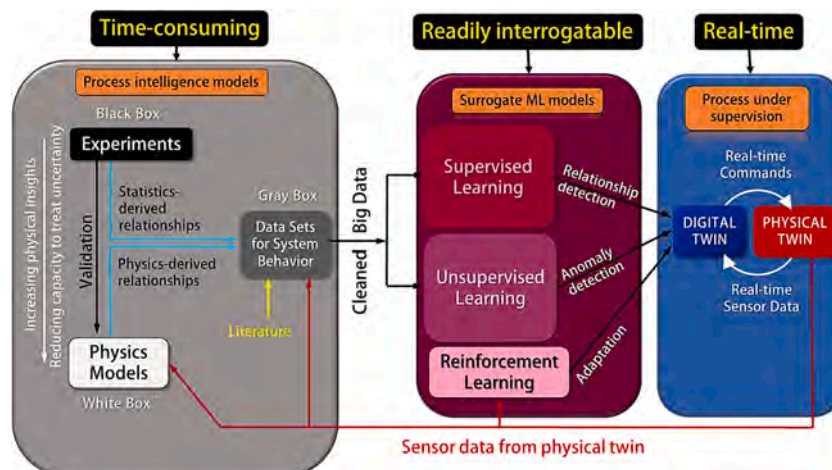

Fig. 2. A simplified schematic of the ecosystem of a process DT.

Such process insights can be coded into a future DT that can act in a supervisory role to ensure the process remains within the desired bounds.

3. The exceptional meshing between AM and DTs

The fit between the DT and AM is extraordinary: AM is full of uncertainty – it produces mostly unique components, each with its individual processing route, and operates in an unstructured and unpredictable environment that is often chaotic, whereas the DT can bring structure and certainty by exercising control. This ability is imparted to the DT through the process insights generated by machine learning (ML) models trained using AM data.

The DT transforms the value of digital data that has been routinely logged since around the 1970s, i.e., since the birth of the microprocessor. Traditionally, these data were used in a limited way: manually visualized and analyzed offline by engineers or scientists to inform future decision-making. They had no bearing on the current state of the process, which may have strayed off-course. By contrast, the DT analyzes the data, extracts insights, and, if necessary, takes corrective action to bring the process back to its desired path, e.g., using multiobjective optimization, all in real-time. The DT is thus analogous to the 'autopilot' that makes a range of autonomous decisions, as found in modern airplanes [42] and some high-end automobiles [43].

This has enormous significance for the manufacturing industry. Since a DT can supervise a process from start to finish using autonomous self-correction so that it doesn't drift from within the desired path, there is the possibility of continually assuring the quality of that process and, by extension, the associated product. This type of anomaly-detecting capability creates the opportunity to avoid rejects, which is a significant benefit to any manufacturing business, but most specifically to an AM business, where each AM build is expensive, making waste also costly. Besides, the increased certainty attached to the integrity of the parts made under supervision can, in time, render destructive testing of the expensive AM parts unnecessary or, at the least, reduce the lot sizes required for such testing – saving time and cost. Finally, the highly dynamic nature of the processes that comprise AM present numerous parameter uncertainties that impinge on repeatability (e.g., see [44, 45]), making diagnostic supervision invaluable. Indeed, the need for process control was identified at a National Science Foundation (NSF) Workshop on *Frontiers of Additive Manufacturing Research and Education* back in 2013 [46]. Process control in AM remains a current topic, as evidenced by a panel discussion on the subject organized in December 2020 by 'America Makes' [47].

Two critical distinguishing characteristics of AM as a manufacturing process are (i) customized parts and (ii) low-volume production. Consequently, parts tend to be unique and of high value. The uniqueness of parts gives rise to situations where the industrial practitioner often has to decide on an optimum processing envelope for a part that has never been made before – and this can result in trial-and-error leading to significant amounts of waste in resources and time. However, if 'what-if' queries were posed to the ML predictive capabilities of a DT or resolved using look-up tables, it would be able to suggest the required processing window quickly. (Therefore, DTs are more than just autopilots). This capability means not only can the part be manufactured sooner, but there will also be much less waste in resources - since trial and error will be reduced or even eliminated. While it might sound far-fetched to some, the use of simulations in the manufacturing industry to get new products right the very first time has been a norm for decades, e.g., see [48]. Although the AM process is harder to predict than conventional manufacturing processes, using reliable virtual models of the process combined with predictive ML algorithms, good quality projections can be obtained. ML-trained feature sets will then become the basis for optimized production.

When acting in a supervisory capacity, the DT provides real-time closed-loop control to rectify anomalies. Three process phenomena are typically monitored [49]: the temperature of the surface of the melt pool and its surroundings, temperature distributions on the surface of entire layers, and the geometric growth of the build. Based on data from such monitoring, the process can be controlled by varying, for example, the power or speed.

At this juncture, we proceed to clarify the difference between the *proactive* control initiated by a DT and the largely *reactive* traditional closed-loop (feedback) control employed in the industry for decades. In essence, the latter is programmed by engineers for known deviations (from the optimal path) with known corrective actions, i.e., using a rules-based approach. Thus, such control is limited to those situations the engineers are already familiar with. However, in the DT scenario, control decisions are made *autonomously* using the vast and up-to-date predictive capabilities contained in the surrogate models, which continually learn from the physical twin. These predictive capabilities allow the DT to foresee a future state of the process, which permits it to take proactive corrective action through what some call *feedforward* loops. This contrasts with traditional *feedback* loops, where remedial action is taken in response to an already encountered deviation on a reactive basis. ML techniques that create the predictive models for DTs can find correlations between cause and effect much more efficiently and use the latest information about the state of the process to update their predictive capabilities. Such expansive and live process intelligence is particularly indispensable for a process such as AM, which is typically influenced by numerous process parameters that often interact with one another in complex ways. It is another reason why the DT concept has a strong meshing with AM. Further discussion on how a DT is superior to traditional closed-loop control may be found elsewhere, e. g., [15].

Clearly, there is a neat interconnection between high-value manufacturing processes such as AM and the DT's use for diagnostic control and process optimization. The ability of DTs to elicit substantial additional returns on investments in AM-related assets and resources is likely to act as a strong incentive for their adoption in the factories of the future. In a recent review that was both comprehensive and in-depth, researchers investigated if and how metal AM will benefit from the introduction of a DT [9]; they concluded that its use would bring down the cost of manufacture of metal AM parts, widening their utility and reach.

In closing, we point out that there could be certain instances where it may not be possible to salvage a deviating AM process using a DT. Such instances can be expected to come to light once a DT is deployed. Some examples of these situations may include process deviations that were not accounted for in the surrogate models or excursions for which suitable corrective actions could not be undertaken. In a similar vein, a closed-loop control strategy cannot be always guaranteed to work. That is simply because, for a control strategy to work, all constituent parts of the system must work as intended. In the case of a sensor failure, for example, a DT may fail to diagnose a process deviation, with undesirable consequences for the quality of the build. Apart from such 'observability' issues, 'controllability' problems may also occur at times. These relate to the inability of the hardware of the AM machine to take an appropriate control action.

3.1. Precursor to DT-controlled AM: demonstration of closed-loop control

In a recent work [18], an open-source laser powder-bed fusion machine (Aconity3D) that can be user-programmed was used to build a stainless steel part. The melt pool was monitored, and pyrometer readings were taken during a series of builds with varying parameters such as scan speed and scan offset. The melt pool dimensions were then manually correlated with pyrometer emission spectra to create a limited database. Similarly, correlations between emission spectra and the scan rate, scan offset, and laser power were obtained and added to the database. Two demonstration builds followed this. In the first build, the laser power was left unchanged throughout the process (indicated by the

horizontal blue line on the top graph shown in Fig. 3). Several hotspots were recorded during the process (Fig. 3, top build), as monitored by the pyrometer. In the second, with the same process parameters, closed-loop control, based on pyrometer readings, was used to change the laser power according to the database's information (blue line on the bottom graph in Fig. 3). In this case, the formation of hotspots was avoided (Fig. 3, bottom build). While demonstrating closed-loop control in AM convincingly, this study relied on manually generated insights into the process. Thus, its scope was limited to the previously investigated process parameters and their boundaries. Also, a considerable amount of time was spent on carrying out the previous set of experimental investigations as well as analyzing data manually to obtain the necessary correlations. It is therefore clear that the study would have benefited from the use of a surrogate ML model enhanced by data from physics models. The ML model would have been able to support many more process parameters and their interactions, providing the investigation with more intelligence to avoid not just hotspots but a host of other defects as well. Nevertheless, this study remains a compelling example of how an AM machine may be controlled in real-time for process improvements. Hence, it may be considered a forerunner to a DT-controlled AM process.

3.2. How collaboration can offer synergistic benefits

We now select another unrelated recent work [49] and show how this work and the one discussed immediately above [18], when considered together, give us a glimpse of how the AM community can move a step closer to applying AI for the betterment of AM.

In the second work [49], laser powder-bed fusion equipment was used to print an H13 steel part. Thermographic images were taken during the metal printing process. These were used to train a convolutional neural network model to detect defects in real-time during a build. The ML model achieved considerable success in the detection of defects such as spatter and delamination. However, no corrective action was instigated on the machine (perhaps because neural networks are 'not interpretable'), unlike in the previous work, to avoid these defects altogether or mitigate their severity. (There are other similar works [50–52] that were conducted in isolation from feedback control of the AM machine.) These works highlight the fact that synergistic benefits could have been reaped had they been conducted under a collaborative strategy, significantly advancing AM R&D.

Fig. 3. The occurrence of overheating (red zones on the top build), and its avoidance (absence of red zones on the bottom build) through real-time control of the laser power (indicated by the blue lines on the graphs). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

4. Challenges to creating mechanistic models for metal AM and potential solutions

Here we outline the technical and non-technical barriers separately. While modelers have considered many of these challenges in the past, we briefly re-examine them from an AM viewpoint. The list provided here is not by any means exhaustive, nor is our treatment of the subject comprehensive. Instead, we hope that, at the very least, the current dialog will catalyze more in-depth discussions on establishing research directions and tackling open questions, with the ultimate aim of commencing a collaborative modeling effort on a global scale. We echo the previously articulated view [53] that genuine cooperation between research communities at large is not only possible but also highly desirable, if not essential, because of the intrinsically multi-disciplinary nature of advanced physics-based modeling.

4.1. Technical barriers and potential solutions

High-fidelity simulations of the various aspects of the AM process are required to generate data sets that can be used for the training of ML models. Since the simulations must be accurate and reliable, all critical influencing factors must be taken into consideration, each at a suitable level of resolution. This requirement represents a challenge, insofar as present-day computer hardware capabilities are concerned, in terms of the timeframes required for obtaining solutions; even in the current era of petascale computing. Thus, ways must be found, using smart approaches drawn from mathematics and domain expertise, to obtain acceptable solutions within reasonable times. Software schemes that can handle the sheer complexities of the sub-processes that constitute AM and link the different sub-models are also required. In addition, strategies are needed to quantify (and limit) the uncertainties contained in the models using, for example, experimental or field validation. Technical challenges such as these are addressed in this Section, and potential solutions are discussed. While some issues, such as creating a common framework and agreeing on standardized methods, are best tackled at the outset through strong global leadership, other subjects may be progressively addressed.

4.1.1. Deficiencies in modeling of AM at a single scale
Before the multiscale and multiphysics questions are addressed, it is useful to take stock of the deficiencies encountered in presently available single-scale, single-physics models of AM sub-processes, which together constitute the collective AM model. Some existing drawbacks and solutions are discussed below.

4.1.1.1. Current dependence on commercial codes. King et al. [35] identified that commercial codes, which are essentially 'black boxes,' have been used for the vast majority of AM simulations. The lack of transparency in those codes (which usually do not support open-source coding) would not only prevent the incorporation of optimal algorithms that would enable more realistic and efficient computations but also limit the possibility of linking the models seamlessly to account for interactions between the sub-processes. Using in-house codes, where the user has total control, is the best option in terms of building flexibility into models. Using an object-oriented language such as C++, it is possible to modularize a problem into separate functions that can be linked subsequently to provide a full simulation. Some institutions are better equipped than others to develop in-house codes. However, since few groups can produce such a comprehensive suite of codes and since all groups have strengths and weaknesses, a shared approach (or a barter system) is preferable. An open-source modular framework that can accommodate various such in-house modules is an attractive but challenging proposition. It must be able to accommodate disparate codes (operating at different scales and solving governing equations rooted in diverse physics) through the provision of efficient linkages. Such
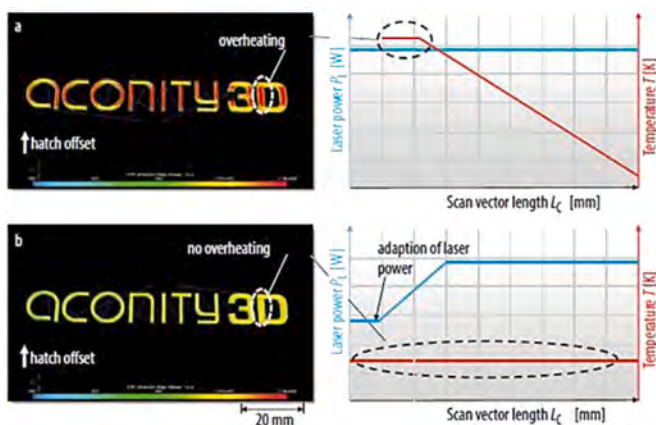
communication should occur without unacceptable losses in resolution across boundaries, which can become sources of error during the transfer of data. Existing examples of such frameworks (e.g., from the Exascale Computing Project (ECP) [54]) that could be adapted for AM are discussed later in Section 4.1.2.1. It must be borne in mind that creating an open framework source usually requires web support and funding to maintain it. We refer to similar efforts (e.g., nanoHUB [55] funded by the NSF to host a large number of programs, apps and codes for use by the public) that have been instrumental in the past for creating and sustaining collaborative resources.

4.1.1.2. Shortcomings shared with other physics-based models. These include, but are not limited to: (i) simplifying assumptions that are usually made to improve the efficiency of computation and/or account for unknown influences, (ii) lack of accurate input data (e.g., material properties at elevated temperatures) and (iii) the dearth of experimental or field data for validation. One way of tackling these problems is to find out the sensitivity of any process route to a range of parameter values (e. g., laser power, scan rate) to find the 'critical few' influences from the 'trivial many.' This can be done either computationally or using controlled experiments. The 'design of experiments' method [56] provides an option for limiting the number of physical and/or numerical experiments required in some situations. Care must be taken to interpret correlations, as a high correlation does not always imply a strong causal relationship. Having fewer relationships (i.e., fewer "features") may bestow the additional benefit of reducing the likelihood of overfitting a trained model, especially when data are limited – making it more generalized and, therefore, a more accurate predictor. Once the vital parameters are established, modelers need to expend time and resources only in finding accurate information for those stronger influences. This focused approach can also be used to design targeted experiments and/or selective logging of field data to expand AM domain expertise and broaden the data set for the training of ML models. The generation of good quality input data, including missing material property data, is resource-intensive, so sufficient funds need to be made available to researchers.

4.1.2. Challenges posed by the multiscale nature of the process

The main objective of multiscale modeling is to identify and establish causal relations between data [57]. Metal AM is a multiscale process and thus must be modeled as such. Furthermore, LPBF is a collection of sub-processes that are governed by different physics (as discussed in more detail in Section 4.1.3). All the relevant physical processes need to be accounted for so that their influences are adequately captured. Requirements such as these create various hurdles, which are considered below.

Powder-bed metal AM (Fig. 4), described in good detail elsewhere [58], is the sum of sub-processes that happen at multiple length- and time-scales, making it a multiscale phenomenon.
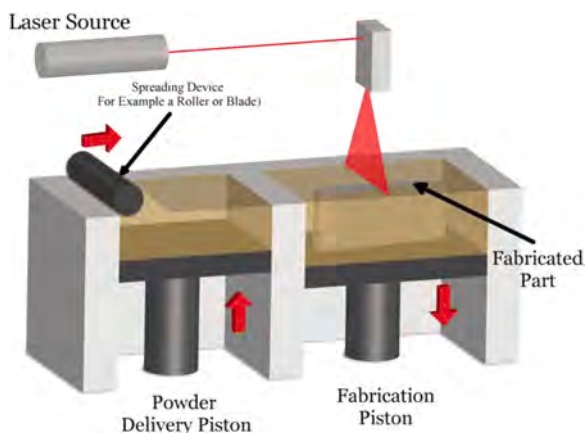
The AM process starts with near-spherical metal alloy powders around tens of micrometers in diameter as raw material and ends with a finished product of usually a few centimeters in size. In-between, complex laser-material interactions drive powder melting and the development of a dynamic melt pool (tens to hundreds of micrometers) occurs, followed by solidification resulting in microstructure formation (nanometers to micrometers). The finished build can often experience distortion due to the relaxing of residual stresses after the part is removed from the build plate, a phenomenon that is usually described in the continuum (macroscopic) scale. Thus, modeling the AM process as the sum of the various sub-processes that are performed sequentially and/or simultaneously obviously becomes a multiscale problem. To add to the complexity, sub-processes influence each other and these interactions may be two-way couplings (Fig. 6). Note that, to preserve clarity, not all inputs that are associated with each of the sub-processes are shown. For instance, the melt pool model will need to have information relevant to the heat source (e.g., laser power, laser spot size, laser scan rate) and heat loss rates (e.g., the flow rate of the cover gas which may remove some heat from the pool through forced convection). In addition, in the graphic we have disregarded potential influences from upscale processing such as recycling powders for reuse [60] (Fig. 5).

At the core of a multiscale model are sub-models and the algorithms that couple together processes at different scales. The latter transform information at one scale and transfer it to another scale in a process known as 'scale-bridging.' Methods used for such bridging include sampling, projection, splitting, lifting/upscaling, homogenization/coarse-graining, refinement, micro–macro coupling, constitutive models, and boundary methods [53,62,63]. Computational challenges relating to the multiscale modeling of AM are not dissimilar to those encountered in other multiscale processes. Some major issues for AM in this category are discussed below.

4.1.2.1. Linking strategies – framework. An important question for multiscale modelers of AM is whether they can reduce the various scale-bridging methods prevalent in the field to a few generic classes that can be linked efficiently, bi-directionally, and without unacceptable loss of accuracy, within a single, over-arching framework. Citing past works in other fields, experts have suggested this is possible and, importantly, can be independent of the process being modeled [53]. However, it is not likely to be cost-effective for the AM modeling community to reinvent a multiscale modeling framework. Rather, the focus should be on evaluating the currently available generic versions and adapt the most suitable. Notable examples include the US Army Research Laboratory's package [64] as well as the EU's Multiscale Modeling and Simulation Framework (MMSF) [65]. For instance, in MMSF, which has been successfully adapted for a range of disciplines [66] including biology, nanomaterials, and hydrology, the single-scale models and their couplings are specified with a Multiscale Modeling Language (MML), which forms the backbone. It describes the scales and computational requirements of sub-models and any scale bridging components that are needed. A coupling library such as MUSCLE2 [67,68] or HMS [64,68] is
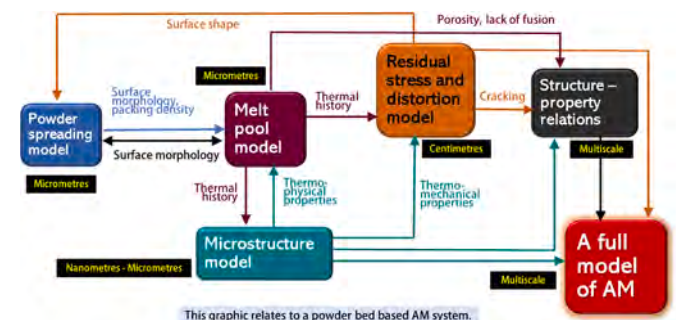

Fig. 4. An illustration of the laser powder-bed process [59].

Fig. 6. A graphic illustrating the multiscale nature of the AM process [61].

Complex Physics

- Heat and Mass transfer
- Wetting
- Melting and solidification
- Fluid dynamics in melt pool
- Grain growth
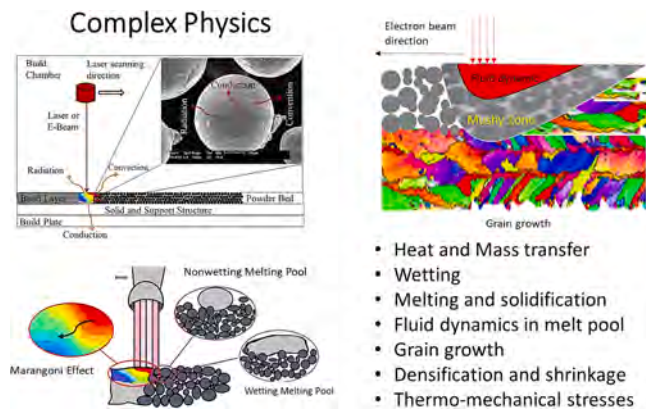- Densification and shrinkage
- Thermo-mechanical stresses

Fig. 5. Interactions between single-level sub-processes that make up the powder-bed AM process. The length scale of each sub-process and the potential methods by which it may be modeled are also shown. Other inputs such as process parameters and thermo-physical data have been left out to preserve clarity.

then used for the communication between the heterogeneous components. MUSCLE2 is flexible enough to incorporate model components written in a variety of programming languages, including Java, C, C++, Python, and Fortran, and can directly generate runtime configurations using the MML specification of a multiscale model. Sub-models are executed on diverse computing infrastructure. An important aspect of MMSF is that it is continuously improved; efforts are presently underway to update its algorithms for the emerging exascale computing architectures [65,69]. MMSF can accommodate legacy and new codes and has also been shown to able to accommodate lower scale (atomistic- and molecular-dynamics-based) models [70]. This is also important for AM since we must allow for the eventual integration of lower scale models to investigate, with increased detail, microscopic phenomena such as the melting and fusion dynamics of powders on a powder bed, e.g. [71].

4.1.2.2. Linking strategies – intermediate surrogate. It has been shown that, in at least some cases, the use of a physics-agnostic surrogate model between two single-scale models can substantially reduce computation times [72,73]. Thus, it may be prudent to investigate the use of surrogates for scale-bridging, and even physics-bridging, scenarios. One must, however, be aware that the cost of constructing intermediate surrogates may be high, given the amount of data that is usually required [74]. Therefore, it is worth examining strategies (e.g., use of the sparse Gaussian process regression method) that have been proposed to overcome such barriers. This method has been used already within the AM community to predict porosity in metal-based SLM [75]. An intermediate option is reduced-order models, which use lower-dimensional projections of the full-order models [76] in which the conservation of mass, momentum, energy, and species is usually ensured. The reduced-order versions can be significantly more efficient than full-order models while retaining some of the physics.

4.1.2.3. Linking strategies - error estimation and propagation. 'Coarse-graining' (or averaging or homogenization) is implemented in order to reproduce critical quantities at larger length and time scales [77]. This, in turn, extends the modeling to a wider scale range at an affordable computational cost. However, the approximations involved in passing information from a lower scale to a higher scale produce an error below some threshold. In some cases, this scale-coupling is required to be two-way, resulting in further error propagation owing to insufficient resolution during downscaling. Therefore, it becomes necessary to quantify these uncertainties, along with those inherent in the inputs (see Section 4.1.8 for a discussion on this), to have a known level of confidence in the predictions. To gain control over error propagation, the

modeler must first have the ability to estimate the error. For example, the error analysis strategy used in connecting a molecular scale model with a continuum scale model through a surrogate [78] may be considered. The modeling error was defined as the difference between the solution of a reference particle model, which was considered intractable due to the numerous degrees of freedom at the scale, and the solution of a manageable multiscale surrogate problem. The method relied on computable estimates of the modeling error in specific outputs of interest, which required the solution of an 'adjoint problem'. These were the so-called 'goal-oriented error estimates', which were used to adapt the surrogate model, i.e., to find the optimal configuration of the overlap region between the molecular and continuum models, in order to deliver approximations of the quantities of interest within some preset accuracy. A detailed examination of the treatment of errors in multiscale modeling may be found elsewhere [79].

4.1.2.4. Linking strategies – mathematics. Since the mathematics used for various sub-models is intrinsically linked to the underlying physics and, consequently, the domain discretization scheme used, it is necessary to address the numerical 'handshake' between the sub-models properly. This becomes a more challenging task if there is two-way communication between the models because the scheme needs to not only ensure sufficient accuracy is preserved, but also must be efficient. The common framework discussed in Section 4.1.2.1 is a potential solution. The algorithms used must ensure that the number and severity of propagated errors are kept to a minimum. Hence a suitable balance must be struck between the computational burden and the degree of accuracy, with the adequacy of this balance decided preferably through an aptly defined quantitative measure, accepted by the AM modeling community, to ensure uniformity. This measure could take any form, but a reasonable starting point could be to base it on quantified uncertainty (see Section 4.1.8).

4.1.2.5. "Enhancing" multiscale models using ML. The use of ML for creating surrogate models has been mentioned previously (Section 2) and will be discussed in detail in Section 4.1.10, along with other ML-derived solution speed-up strategies. However, a relatively new school of thought merits a brief mention here. It has been suggested that ML and multiscale modeling can naturally complement each other to create improved predictive models that integrate the underlying physics to manage ill-posed problems and explore "massive design spaces" [57]. The proponents of this thinking argue that, once the ML models have learned from data, these models themselves become superior to the sources from which the data were obtained, namely multiscale models as well as experimental and field data. That is because, even though the ML models are physics-agnostic, the AI contained within them is associated with the gray box (Fig. 2), rather than the white box (physical data) or black box (model predictions) alone – so, the black box data is validated by the white box data and vice versa. They also point out that multiscale modeling alone often fails to efficiently combine large datasets from different sources and different levels of resolution. Similar thoughts have been offered recently [80] on the potentially symbiotic relationship between multiscale models and ML models. The latter authors point out that multiscale models can benefit from ML models, which are superior in their handling of ill-posed problems (which computational models struggle to solve), and in the management of noisy data. On the other hand, multiscale models can integrate ML to create surrogate models, identify system dynamics and parameters, analyze sensitivities, and quantify uncertainty, to bridge the scales and understand the emergence of functions. It has also been suggested that we can use ML to quantify the agreement between correlated data, for example, by comparing computationally simulated and experimentally measured features across multiple scales using Bayesian inference and uncertainty quantification [81]. In our context, therefore, it is useful to explore the possibility of linking disparate models via the use of ML

mechanisms – especially if connecting through mathematics or algorithms proves challenging or impossible. Care must however be taken to ensure that the hybrid approach does not inadvertently amplify the flaws, artefacts and/or biases attached to the ML or physical data.

4.1.3. Hurdles created by the multiphysics nature of the AM process

Superimposed on the multiscale nature of AM is the interplay of multiple physics that governs the sub-processes – see Fig. 6. For instance, consider powder coating (raking) in the powder bed, and powder melting, where the physics involved is mechanics and heat transfer/fluid dynamics, respectively. Additionally, microstructure formation is dictated by thermodynamics and mechanisms such as nucleation. Hence models describing these sub-processes have their individual governing equations, which are solved differently based on the formulation strategy and the discretization scheme used. It then becomes a challenge to pass information between the various models to account for the frequent interactions that happen between the sub-processes.

The dissimilarities in codes between treatments of multiple scales and multiple types of physics have much in common. Therefore, several of the challenges and solutions discussed in Section 4.1.2 for linking disparate multiscale models apply equally well to connecting distinct physics models. Furthermore, in a recent article [76], the challenges of multiphysics modeling in metal AM have been dealt with in some detail. That article also points to some comprehensive reviews of related subjects. Another recent publication has reviewed a collection of methods used for modeling AM [82]. Therefore, we limit ourselves here to aspects not covered elsewhere in the AM-related literature.

4.1.3.1. Linking strategies – integration of disparate physics.
As can be seen from Fig. 6, a variety of computational methods is used for the single-scale models – all of which are required to be linked one way or another to create the end-to-end AM model. The framework discussed previously (Section 4.1.2.1) for multiscale 'numerical handshakes' could be adapted for use in linking multiphysics models as well. Besides, it is worth drawing from tested concepts that underpinned attempts at connecting diverse models – some of which were incidentally from within the AM discipline itself. In a recent such work [76] that modeled the laser cladding process, either a reduced-order model was developed from a full-order model to overcome the problem of finding a suitable method for solving equations from different physics, or alternative approximate approaches for solutions were proposed. The complementary methods proposed were not without their drawbacks, however, as the authors themselves acknowledged.

4.1.3.2. Linking strategies – development of a common algebraic coupling paradigm.
Some experts have called for a complete re-think of multiphysics coupling strategies that can take advantage of new and powerful computing environments. In a seminal work [83] entitled 'Multiphysics simulations: challenges and opportunities' written by over forty global experts in the field, the authors tackled the multiphysics modeling issue holistically. They considered multiphysics applications from algorithmic and architectural perspectives, where "algorithmic'' included both mathematical analysis and computational complexity, and "architectural'' included both software and hardware environments. According to the publication, researchers have already made substantial progress in understanding coupling issues for multiphysics components, including aspects of problem formulation, discretization, meshing, multidomain interfaces, interpolation, partitioned time-stepping, operator-specific preconditioning, as well as have a good understanding of difficulties that can arise in multiphysics operator decomposition. The experts concluded that new mathematical tools and computational approaches were prerequisites to ensure that coupling schemes are accurate, stable, robust, consistent, and are implemented correctly, for developing predictive multiphysics simulations.

4.1.3.3. Accounting for physical phenomena specific to AM.
There are several characteristics unique to powder-bed AM processes. An example is the use of raw material in the form of powders that are only tens of micrometers in diameter. The powder packing density in the bed can have an influence on the part properties [84]. Hence, unless the powder coating is simulated accurately, the resulting predicted part properties may not be correct. While similar to laser welding, the relatively high scan velocities and small laser spot size create a dynamically evolving melt pool that is particularly susceptible to keyhole-driven defect formation. Other examples are the distinctive microstructures created through rapid solidification and the relatively high residual stresses found on the built parts. These are attributable to the large temperature gradients and cooling rates that develop on the component being built, as the heat contained in the minuscule nascent melt pool is rapidly diffused away into either the substrate or the previously solidified layers. Hence, all the physics involved in this interplay must be given sufficient consideration. However, until the relevant processes are well understood to be modeled deterministically, a phenomenological approach (based on experimental results) can be used. If sufficient experimental data is available, ML models may be trained for the purpose given the greater efficiency with which these can uncover potential correlations.

4.1.4. Verification – challenges from interactions between sub-processes

Verification is the process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model [85]. Verification, therefore, is about confirming that the equations in the models were solved correctly (Fig. 7). A summary of the verifications that need to be carried out is provided in Table 1.

Verification is a requirement common to all modeling efforts – not just those within AM. However, the fact that the AM process is a sum of several sub-processes that operate at multiple scales while being governed by multiple physics complicates 'calculation verification'. This is mainly because of the several interactions that occur between the sub-processes (Fig. 6), which often need to be accounted for. Nevertheless, a systematic attempt is required to ensure the reliability of the sub-models, and, by extension, the full model. The subject is dealt with in detail in Reference [85].

4.1.5. Validation – barriers for the generation of experimental data

Validation is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model [85]. Experimental validation of model predictions is necessary to increase the practitioners' confidence – and hence reliance - in the models. Also, validation assists the modelers to
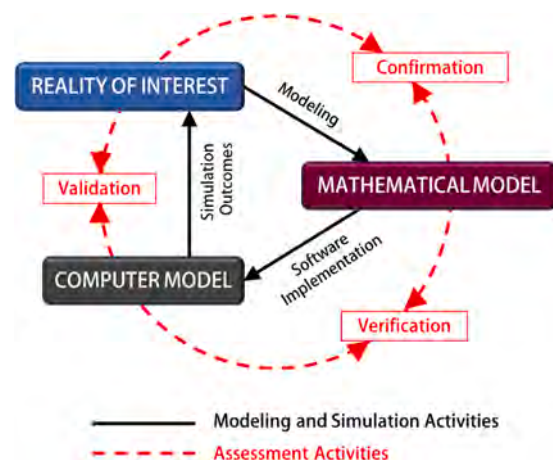

Fig. 7. Simplified view of the model verification and validation process [86].

Table 1
Verification assessment classifications [60].

Classification		Focus	Responsibility	Methods
Code Verification	Software Quality Assurance	Reliability and robustness of the software	Code developer & Model developer	Configuration management, static & dynamic testing, etc.
	Numerical Algorithm Verification	Correctness of the numerical algorithms in the code	Model developer	Analytical solutions, benchmark problems, manufactured solutions, etc.
Calculation Verification	Numerical Error Estimation	Estimation of the numerical accuracy of a given solution to the governing equations	Model developer	Grid convergence, time convergence, etc

quantify the adequacy of their assumptions (relating to physics, material properties, etc.), choice of numerical resolution, algorithms, mathematics, and the like. The models are assessed using what is called a 'validation metric,' which is a predefined measure that agrees on the level of accuracy and precision of a simulation. The experimentally obtained data must be of high quality and generated under rigorous, tightly controlled conditions. All assumptions in the model being validated ought to be understood, well defined, and controlled in the associated experiments [85]. Once obtained, this data is transformed using uncertainty quantification to obtain experimental outcomes, which can then be compared with simulation outcomes (Fig. 8). The quantitative comparison of experimental and simulation outcomes may take the form of a statistical statement of the selected validation metrics. For instance, if the validation metric were the difference between the simulation and experimental outcome (or simply "error"), the quantitative comparison would quantify the expected accuracy of the model, e. g., "We are 95% confident that the error is between 5% and 10%."

The problem is that carrying out controlled experiments in AM is not easy, given the dynamic nature of many of the sub-processes (e.g. powder coating) and the chaotic, unstructured nature of the laser-powder-melt pool interaction. For instance, where the laser interacts with the metal powders being melted, there is a host of complex, dynamic phenomena that happen: powder spatter [87], keyhole formation at high energy densities [88], fluid dynamics governed by Marangoni effects [89,90], droplet ejection and melt-pool surface

depression/protrusion [91], vaporization [89,90], and the like. Also, because some of the sub-processes proceed at a rapid pace in tandem with the extremely high laser scan rates, observing the process is not easy. Further, because the nascent melt pool is microscopic, the equipment needs to be of a high-resolution, apart from being capable of high-speed image capture (i.e., tens to hundreds of kHz frame rates), for observing crucial aspects of the process, e.g., the temperature evolution, and elucidate the physics of denudation, spatter, entrainment [92,93]. While such hurdles create the need for high-end, expensive hardware, several successful attempts have been already made to gain a deeper understanding of the process, and thereby unlock the underlying science. Examples of these include advanced CMOS (complementary metal-oxide semiconductor) video camera to study spatter and melt dynamics [91]; high-energy X-ray imaging technique to investigate the dynamic powder scatter mechanism [87]; in-situ X-ray synchrotron experiments to capture fast, transient dynamics at the meso-nanosecond scale [41], and in situ X-ray imaging to study the mechanism of pore formation and liquid-solid interface dynamics [88]. In the latter two works, researchers used multiphysics simulations to reconstruct the processes involved and, subsequently, to determine optimum process conditions. It is thus apparent that high-quality experimental data is progressively reaching the open domain, making it possible for modelers to increase the accuracy and resolution in their models.

A significant challenge in this category arises from the fact that several alloys and compositions, as well as numerous process
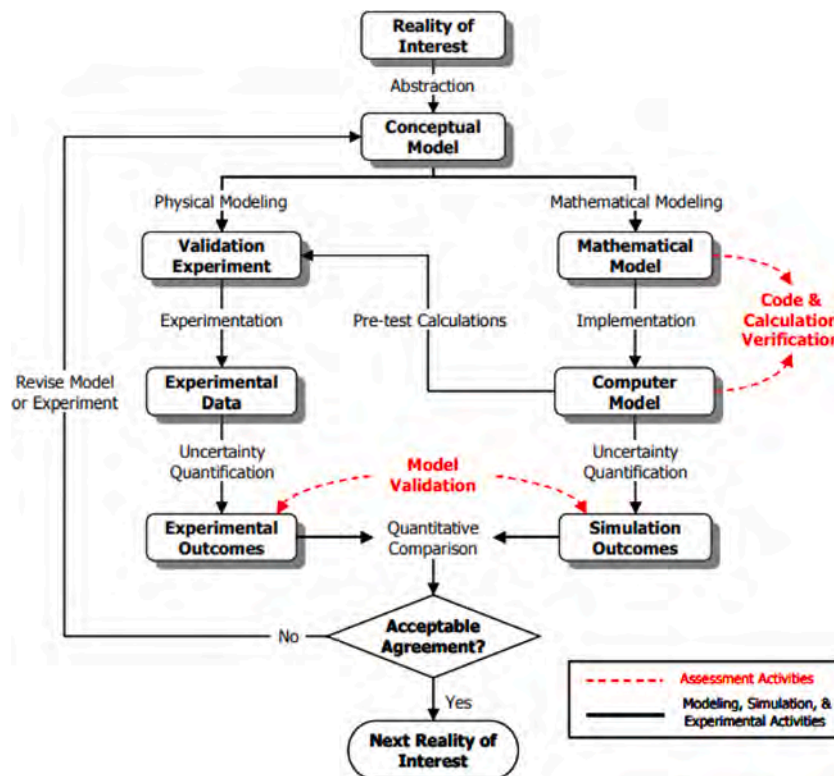

Fig. 8. Model development, verification and validation [60].

parameters, are used in AM. For instance, more than 100 independent process parameters are involved in a typical powder-bed AM process [94]. This results in a massive number of permutations and combinations of materials and processes. Hence, in any collaborative effort, a manageable number of combinations may be selected by consensus. In the open domain, there already appears to be natural gravitation towards alloys that are of the highest commercial interest, e.g., Ti6Al4V, AlSi10Mg and stainless steel 316. Therefore, in selecting the materials systems, pragmatic considerations can provide guidance. Not coincidentally, these alloys are amongst those 'most weldable.' However, there is a need, still, to develop a broader set of alloys better suited to AM (i.e., rapid solidification) environments.

4.1.6. Generating inputs for models – the need for a focused approach

As with validation data (Section 4.1.5), the generation of model inputs requires a consensus approach from the community. The reason is the same: there is a huge diversity in alloys and process parameters. Again, it will be useful to identify a handful of these for a focused investigation. The Phenomena Identification and Ranking Technique (PIRT) may be of use here in prioritizing research. It is a systematic way of gathering information from experts on a specific subject and ranking the importance of the information in order to meet some decision-making objective, e.g., determining what has the highest priority for research on a given subject [95]. An important part of the PIRT process is to identify the uncertainty in the ranking, usually by scoring the knowledge base for the phenomenon. The rationale for the scoring is an important product of the elicitation. When a phenomenon is identified as important, but the corresponding knowledge level is low, more effort must be directed at it, e.g., more research support.

A common understanding is also necessary within the community on the amount of rigor that will be attached to the models. That would determine the quality and quantity of data that will be sought for the development of the models.

Saving all information developed, as well as gleaned from the public domain, in an accessible, well-organized, and easily interrogatable database would facilitate efficient data exchanges.

4.1.6.1. Material properties.
It is well-known amongst modelers that most thermophysical properties are a function of temperature and finding reliable values is difficult, especially at elevated temperatures. It becomes even more challenging for properties that may be esoteric, e.g., the coefficient of friction between the powders on a powder bed. While some large multinational corporations may have these in their private collection, only limited information is available in the public domain. Therefore, a global collaborative endeavor is necessary to fill in the vacuum. Groups involved in the generation of the properties must agree to standardized methods (Section 4.1.8), including on how best to quantify uncertainty (Section 4.1.7). While there are copious different compositions that have been additively deposited, and the number of AM alloys are more numerous than those used for traditional processes such as casting or welding, any collaborative work must prioritize a selected number of alloys.

4.1.6.2. Boundary conditions (BCs).
These allow us to limit our space of interest in modeling to only the most crucial regions, which saves computational cost. They prescribe values at every point on the boundary of that space to quantities that vary throughout a given space or enclosure. Solutions of the partial differential equations for the quantities close to the boundary will be more strongly influenced by the prescribed values than for those in volumes remote from the boundaries. In some cases, however, BCs can influence the solutions for the entire region of interest. It is, therefore, crucial to collaboratively decide on the treatment of various BCs, as discussed for material properties above (Section 4.1.6.1). If there is high confidence in the accuracy of BCs, the size of the computational domain may be reduced – since there would be little or no undesirable influences on the solutions within the domain – with concomitant gains in solution times. The introduction of BCs do, however, create a series of problems during feature extraction and can subsequently have a significant and negative effect on ML if not characterized correctly.

4.1.7. Uncertainty quantification for an inherently random AM process

There must be uniformity in how uncertainty is defined and treated. Uncertainty is described as a potential deficiency in any phase or activity of the modeling or experimentation process that is due to inherent variability (irreducible uncertainty) or lack of knowledge (reducible uncertainty) [85]. Therefore, 'uncertainty quantification' (UQ) is the process of characterizing all uncertainties in the model and experiment, and quantifying their effect on the simulation and experimental outcomes. Note that, in Fig. 8, UQ is mentioned in both the experimental and simulation branches. Meticulous UQ is a prerequisite for meaningful validation, which is the assessment of if - and to what degree - the results of a simulated model can be trusted to predict reality [96].

Uncertainty occurs either due to incomplete, inaccurate or missing data (epistemic uncertainty) or owing to the randomness of the outcome in question (aleatory uncertainty) [69]. Common sources of epistemic uncertainties in experiments include [97]: imprecise definitions leading to multiple interpretations (systematic or random), failure to account for influencing factors (usually systematic), environmental factors (systematic or random), instrument resolution (random), and incorrect calibration of sensors or instruments (systematic). The distinct class of aleatory uncertainty is highly relevant to AM due to the inherent randomness of the process. This can result in different outcomes from a given process for the same set of inputs (process parameters). In simulations, if a model comprises non-deterministic (e.g., statistical) elements to capture the stochastic behavior of a physical process, then one must expect uncertainties attributable to the prescribed randomness. Other uncertainties in simulations can occur due to incomplete, inaccurate or contradictory input data, mechanisms and/or dependencies that may have been missed, subjective 'expert judgments' that may have been incorporated, and a lack of consistency in the modeling assumptions, approximations, and strategies. This is particularly important as knowing the type and source of uncertainty can inform which data science protocols must be followed prior to training any ML models.

In modeling, sensitivity analysis (SA) goes hand-in-glove with UQ [98]. SA is performed to determine the degree to which a solution changes when an input is changed by a pre-determined amount. Thus, SA reveals the inputs that have the most influence, which means a majority of efforts can be directed towards obtaining more accurate information on those crucial inputs. One point to consider is that models can be used for SA reliably only after they are validated for at least a narrow range of parameters around the values of interest.

A recent study [99] has demonstrated the capability of a data-driven UQ framework for the efficient investigation of uncertainty propagation (UP) in the simulation of metallic AM processes. It tackled the UQ from process parameters to material microstructures, and then to macro-level mechanical properties, through a combination of advanced AM multiphysics simulations and data-driven surrogate modeling (see Section 4.1.10). Model correction and parameter calibration for the constructed surrogate models using limited amounts of experimental data were discussed. Thus, the techniques proposed in this work are likely to be applicable in many cases. Another recent work [100] reviewed the research state-of-the-art and discussed needs and opportunities in UQ and uncertainty management of the AM processes (Fig. 9), with a focus on laser powder bed fusion. This study tackled UQ as applied to both experiments and simulations. A further work [101] discussed UQ in the context of multiscale modeling, and explained how errors or uncertainties propagate from one scale to the other. The authors highlighted the lack of an established formal approach in the field. In recent times, the use of ML has been proposed for the task of UQ [102]. It has been suggested that the confidence levels associated with epistemic
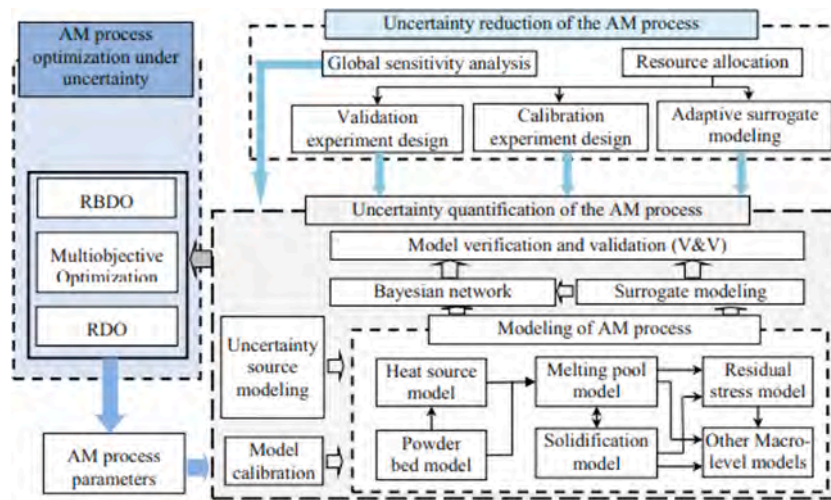
Fig. 9. UQ in the powder bed AM process [73]. Acronyms: RBDO = reliability-based design optimization, RDO = robust design optimization.

uncertainty can be estimated using surrogate models (Section 4.1.10).

It is worth mentioning here that, in addition to uncertainties related to modeling, unique uncertainties are associated with the AM process itself. For instance, the long build times characteristic with metal AM, coupled with system drift and events such as spatter, exacerbate the uncertainties.

4.1.8. Standardization – the need for uniformity in AM modeling

Given AM is a rapidly advancing technology, it is unsurprising that universally accepted standards are not yet available for many of the innovations already incorporated into practice. This situation gives rise to the following scenarios [103,104]: material data reported by various companies are not comparable; technology users employ different process parameters to operate their equipment according to their own preferences; there is little repeatability of results between the system suppliers and the service bureaus; and there are few specifications that end users can reference to help ensure that a product is built as specified. The problem is exacerbated by the several permutations and combinations of alloy systems and process parameters that are employed in AM (Sections 4.1.5 and 4.1.6), and the large array of hardware and software that are used for builds. This gives rise to the following specific issues [105]: standard programming languages (such as G-code and M-code for conventional machine tools) are not well defined, and a method for synchronizing laser power to scan speed does not exist. Furthermore, there is no uniform way of implementing laser scan strategies among AM machine vendors. Customization of scan strategies is, therefore, difficult. Moreover, even with an identical strategy, the build quality could be very different on different machines. This creates great uncertainty in the part qualification process.

Fortunately, the problem has been at least partially recognized. A good example of the progress being made is found in a project [105] funded by the *US National Institute of Standards and Technology* (NIST). In this work, the focus is on developing algorithms, methods and standard protocols for AM process control. Specifically, an open-platform modular AM software will be developed, with all control parameters accessible, and build-in modes to implement typical control methods (with some similarities to the ECP effort [54]). Similarly, a project sponsored by *America Makes* [20] has succeeded in building a set of protocols and a control system that would enable future development of feedforward and feedback control of the PBFAM process. An important player in this space is the *AM Standardization Collaborative* (AMSC) [106], which is a cross-sectoral coordinating body whose objective is to accelerate the development of industry-wide AM standards and specifications. In June 2018, the AMSC published its Standardization Roadmap for AM (Version 2.0) which identified existing and specifications

standards (e.g., by the *American Society for Testing and Materials* or ASTM [107]), as well as gaps.

Historically, in 2009, ASTM started F42 Committee for developing standards for AM. In 2011 ISO formed the ISOTC261 committee that is focused on the same. In 2013, both ASTM and ISO came together to form a joint plan. More details on their contributions may be found in [61]. However, modeling and simulation of AM have not been addressed. The closest attempt, so far, to tackle the topic appears to be the creation of the ASME *V&V Subcommittee 50, Verification and Validation of Computational Modeling for Advanced Manufacturing*, to provide procedures for verification, validation and uncertainty quantification in modeling and computational simulation for advanced manufacturing [31]. The AM modeling community can borrow from the recommendations of this committee. Consistency in modeling between the various groups can substantially accelerate the pace of model development, as it would allow for efficient data exchanges and facilitate modular development of sub-models that can, when combined, comprise a full model of AM.

The need for standardization in manufacturing has been well recognized for a long time. However, adoption of and adherence to the standards can be encouraged by industry associations and even mandated by legislation. National bodies tasked with the oversight of standards have an important role to play in this area.

4.1.9. Acceleration of solution speeds – hardware and software techniques

Physics-based computational models stand to benefit from an increase in solution speeds. This is because of the relatively long durations ('wall times'), typically hours or days, required to arrive at solutions. Speed-up may be achieved through hardware, software, or both. Further exponential increases in solution speeds can be achieved by the creation of reduced-order 'surrogate models,' discussed in Section 4.1.10.

Hardware acceleration is now commonplace in high-performance parallel computing, where supercomputers or clusters of computers make scientific computations solvable within much shorter timeframes. Since scientific computing and graphics processing both involve the same floating-point operations, General Purpose Graphical Processing Units (GPGPUs), Tensor Processing Units (TPUs) and Field Programmable Gate Arrays (FPGAs) are increasingly used for achieving higher computational speeds in science. In addition, network hardware (e.g., Infiniband) is also evolving rapidly to support increased communications speeds. There is little doubt that modelers in the AM community will benefit from suitable hardware infrastructure.

However, acceleration using hardware is only part of the picture. Modern software codes must not only incorporate their unique innovations, but should also be able to take advantage of the new efficiencies offered by the rapidly improving hardware capabilities.

Recognizing this important point, a group of workers has offered a series of thoughts on how multiscale high-performance computing could be conducted in an exascale computing era using advanced coding [65,69, 72]. It is now accepted that significant code refactoring is needed to take advantage of new hardware and there are entire programs within the United States Departmnent of Energy Exascale Computing Project (ECP) [54] dedicated to rewriting algorithms from scratch – because it is not just a matter of changing to a new language. The software structure and algorithms of GPU codes is entirely different to CPU codes, and the structure of the chips are different. Heterogeneous hardware is one of the biggest challenges facing the HPC community at the moment.

Modelers within the AM community are conscious of the need to make their approaches more efficient. Multiscale modeling itself is a coarse-graining technique that saves computational time. Adaptive meshing is another method whereby mesh densities at regions away from the current region of interest are coarsened. This is of particular relevance when simulating layer-by-layer deposition since the melt pool is microscopic, but the final part is large. Finer mesh densities in and around the melt pool zone capture the extreme thermal gradients and fluid dynamics while a comparable computational cost is not carried by remote regions. Adaptive meshing has been demonstrated in AM in a thermal-mechanical finite element modeling (FEM) study of an electron-beam-melted part with 107 layers [108].

There are other less widely adopted methods. In a recently published article [109], modelers used what they term a 'meta-modeling' approach for their FEM model. Here, higher-resolution results were predicted from lower-resolution results by applying a Gaussian process-constrained general path (GPGP) model. This is a regression-based approach that interpolates the original solution by considering the influencing parameters, in this case, 'heterogeneous discrepancies.' In addition, there are more traditional techniques at the disposal of modelers. These include suitably approximating non-critical inputs to reduce the number of computations required in a transient simulation – which can result in significant aggregate savings over a multitude of time steps.

Finally, a recently proposed and fast-evolving approach is the use of ML to speed up predictions of multiscale models using advanced mathematics [81,110]. In this method, a 'multi-fidelity classifier' is introduced to predict the output of expensive models. This modeling framework relies on a multi-fidelity strategy, which couples the learning progress of the AI with the resolution of the computational models used to generate training data. It trades unnecessary precision of the error gradient used, especially in the early stages of AI training, for computational efficiency. The main objective of the multi-fidelity strategy is to significantly speed up the training of ML models in those domains in which training data have to be generated by means of computational models and where this process constitutes a significant portion of the overall computational cost associated with endowing an AI model with physical intelligence.

4.1.10. ML/AI based surrogate models for real-time solution capability

DTs, when acting in a real-time diagnostic control capacity, need to be able to respond promptly. Such agility is necessary not only for keeping a process from deviating from the preferred path but, if for any reason it already has, to also recover at the earliest. Such urgency cannot be drawn from physics- or statistics-based computational models, which typically take hours or days to solve. Thus, reduced-order, faster-solving ML models, which are 'surrogates' [80] of the original physics or stochastic models, need to be developed (Section 2). The purpose of a surrogate is to reduce the time necessary for a computation at the cost of rigor and generality [111]. These surrogate ML models can be used to detect product and/or process anomalies in real-time during a build, and to determine the optimal processing window - through 'what-if' queries posed to their predictive capabilities – even before a build commences. Because of this utility of ML for the development of DTs, the subject is treated in some detail below. However, the focus is limited to their use in

an AM setting.

A key requirement for creating ML models is a sufficiently large training data set. Since the AM process is relatively slow, and each build is expensive, it is challenging to obtain sufficient data points using experimental methods alone. However, when experiments and validated physics models are used together, it becomes easier to generate the required amount of data (Fig. 2). Therefore, it becomes incumbent on AM technology experts, modelers and ML developers to cultivate a common, standardized understanding of each others' needs as well as potential contributions in the spirit of 'concurrent engineering', and undertake appropriate and rigorous data fusion processes [112].

Before we proceed further, a short primer on associated terminology is provided. To begin with, ML is a subset of the 'catch-all' AI – which may be interpreted to mean "imparting human intelligence to machines" [113]. AI-powered machines are usually separated into two groups — general and narrow. General AI machines can intelligently solve a broad set of problems. Narrow-intelligence AI machines, by contrast, can perform specific tasks very well, sometimes better than humans — though they are limited in scope. The DTs for AM fall into the narrow-intelligence category. ML is a method of training AI algorithms so that they can learn how to perform tasks, the outcomes of which can be used to make decisions when combined with design criteria. Training in ML entails feeding large amounts of data to the algorithm and allowing it to find patterns and learn relationships in the processed information. The difference between traditional programming and ML-derived programming is shown in Fig. 10. Conventional programming is a manual process, where the programmer comes up with the logic (if/then/else) on how a system responds to stimuli (i.e., the rules governing cause and effect). Conventional programming is top-down. On the other hand, in the automated ML process that is 'supervised', the machine (computer) comes up with the rules governing the relationship/s, given the input parameters (including potential causes) and associated outputs (including potential effects) that are aptly labeled by researchers, based on an estimate/improve/repeat logic. For a complex process such as AM, which has numerous influencing independent parameters that can, additionally, interact with each other, the automated method provides the ideal means of modeling. For this, however, one must use the appropriate multi-target regressors, multi-class classifiers or multi-objective optimizers.

A surrogate ML model developed using supervised learning can be used for parameter optimization that helps find an optimum processing route for any given build. This can subsequently be used as the baseline by a supervisory DT, which acts in a diagnostic closed-loop control capacity, to lead the actual build process within specified parameter boundaries.

The most common task for a surrogate ML model developed through unsupervised learning is clustering analysis, in which the output data are separated into groups based on their similarity in a high dimensional feature space. This type of analysis is ideal for detecting anomalies (referred to as outliers), where any deviation from the norm in a small part of the population is recognized. The DT can then act in real-time to rectify the anomaly, e.g., by reducing the laser power to address overheating at a spot. The advantage here is that 'the norm' (referred to as the centroid) need not be predefined; the ML model is able to identify the abnormality for itself based on the data set.

Surrogate models may be built using many ML techniques, including the following regression methods [111,115,116]: support vector
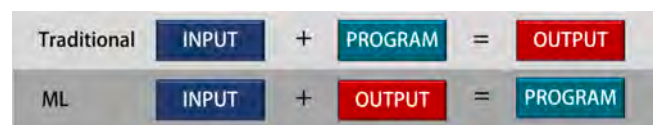

Fig. 10. The difference between traditional and supervised ML-derived programming [114].

machines (SVMs), random forests (RFs), artificial neural networks (ANN), Gaussian process regression, and decision trees. An example of how to build a surrogate model using SVM is found in Reference [111].

ML has been applied already in AM for a variety of purposes, e.g., in microstructure prediction [117–119], to determine the correlation between build parameters and resulting tensile strength [120], materials development [121], and for other purposes [50–52]. Applications such as these and others in the field of AM (e.g., parameter optimization, melt pool temperature and flow prediction, property prediction, defect detection, geometric deviation control, quality prediction, and assessment) were extensively reviewed recently [49,111,115,116,121,122] and categorized [102] into parameter optimization and anomaly detection. These reviews paint a picture of AI just beginning to be used in applications relevant to metal AM. However, in an invited review published recently [121], experts have concluded that AM is positioned to provide foundational case studies for the adoption of ML into physics-based integrated computational materials engineering (ICME), largely due to the simultaneous peak in funding for both AM and data-driven research across the globe. In their view, the success of ML applications in metal AM would provide the foundation for a new paradigm in ICME as a whole.

We conclude here with some considerations relevant to those who wish to create surrogate models (see also Reference [123]). First, an appropriate, interpretable ML technique that is suited for the purpose should be chosen from amongst the several available candidates. The degree of interpretability varies significantly among ML approaches, and is also strongly dependent on the feature extraction, feature engineering, feature selection and any dimension reduction. Most dimension reduction methods and clustering algorithms are not interpretable. The practitioner must be conscious of potential traps in the form of biases in data and learning, as well as data recording errors. This is because surrogate models can inherit, and often amplify, these problems. Possible challenges to creating surrogate ML models are selection bias, evaluation bias, information bias, insufficient data sets, sparsity, missing data, skewed data, imbalanced data, outliers, and difficulties with feature extraction or labeling. One of the most sought-after outputs from ML is the ranking of features (variables) by their influence in predicting labels (outcomes). Highly ranked features are referred to as 'anchors', lower-ranked features are referred to as 'counterfactuals', and unimportant features are 'nuisance variables'. Anchors are used more often in a high-performing model, but each 'use' may represent a small adjustment. Anchors are not necessarily more important to the science than counterfactuals, and can easily be associated with outcomes, rather than driving them. Conversely, a counterfactual may only be used once by the model, but may be pivotal to the AM and have a strong causal relationship.

As much attention as possible must be paid to the available data; it must be cleaned (i.e., modified to ensure that it is free of irrelevant and/or incorrect information), standardized, normalized, stratified (or a sampling method used to handle imbalance), as to exhaust attempts to extract as many features as possible from the data to avoid evaluation bias. All hyper-parameters should be optimized every time the data set changes. Models should be cross-validated and tested on unseen data, and evaluated for accuracy generalizability and, if undertaking classification, precision, and recall. Then the outcomes must be compared with experiments to interpret them in context with relation to domain knowledge.

4.2. Non-technical barriers and potential solutions

As shown by an example given in Section 0, a combined effort is likely to be more fruitful than insular efforts. Similarly, synergies resulting from wider alliances are likely to be larger than from collaborations conducted on a limited scale. However, any proposed large-scale collaborative research effort comes with its own distinctive challenges, quite apart from the technical hurdles considered earlier (in

Section 4.1). Added complexities are introduced by the geographically dispersed nature of the potential participants and the different goals that each stakeholder (e.g., industry, academia, research laboratories, government) is, by organizational design, positioned to pursue. Also, convincing funding bodies may become a challenge particularly if they have preconceived ideas or strict government directives that are perceived to run counter. Identifying these obstacles and finding consensus and compromise within the AM community to overcome them is, in our view, a useful first step. We therefore flag here some of the issues that need to be collectively addressed and offer some thoughts on potential paths forward.

4.2.1. Creating a shared global vision

A common goal that is centered around the betterment of AM is an ideal starting point for any international collaboration. It comes with the recognition that AM, as an enabling technology, has a vast potential to not only make manufacturing more sustainable through reduced waste, but also to help manufacture products that result in better performance (e.g., improved fuel efficiency). While canvassing universal support for the cause is unlikely to be an easy task and will require strong global leadership and dedication, a number of committed groups could nevertheless be expected to sign up to take advantage of the synergies on offer. A key aspect of garnering voluntary participation will be to articulate clearly the increased benefits each stakeholder is likely to enjoy in return for being part of a coordinated effort.

4.2.2. The need for coordination

The presence of an overarching coordinating body is likely to make the collaborative effort more workable by creating the necessary framework that provides the infrastructure for interactions and includes rules of engagement. An obvious example is the *America Makes* initiative [124], although its outlook is national rather than international.

Some organizations are more suited to providing genuinely international leadership. For instance, the US-based Minerals, Metals & Materials Society (TMS) or the UK-based Institute of Physics (IOP) have memberships from around the world. However, participation of at least some national organizations that have the clout and capacity to contribute is likely necessary for the success of any efforts. Examples of these bodies include, but are not limited to: NIST, NSF, ANSI, AMSC, ASTM, ASME, universities worldwide and government laboratories in the US and elsewhere - such as Fraunhofer in Germany, A*STAR in Singapore, CSIRO in Australia, and Chinese Academy of Sciences – and societies such as European Factories of the Future Research Association and MAKE UK.

4.2.3. Deciding on the type of partnership

The AM community may need to decide up front if the collaboration would be on a non-cash academic basis where each volunteer member contributes to research at their own cost, or if it would be a legally-binding pecuniary arrangement that allows subcontracting between participants. It may be possible to have a hybrid approach, where the latter is allowed between interested parties.

4.2.4. The challenges of industry-research partnerships

While useful to obtaining a line of sight for commercializing research and gaining a sense for market demand as well as funding, creating a robust and symbiotic partnership between the industry and academic/government research organizations is a major hurdle for a number of reasons. Chief among these is the misalignment of reward systems in the two sectors: pecuniary in the commercial world vs. knowledge dissemination in research. Embedding researchers within industry may help with understanding and communication, besides developing a shared goal. In addition, one of the main requirements for making modular model development succeed, viz. use of open-source codes, may obligate the sharing of work to outside parties if those codes were distributed under GNU licensing protocols [125]. This may have the effect of

eroding the competitive advantage of industry participants of the collaboration. It is however likely that the industry will obtain a return far above what they invest into a collaboration, and analyzing this further and quantifying it is likely to assist in obtaining buy-in. One way of protecting participating commercial interests is to patent significant inventions before publishing, and then offer the rights to those patents either royalty-free or on a discounted basis.

4.2.5. Fair treatment of intellectual property, data protocols and data sovereignty

The research community may have to be prepared to delay publications until after patenting if they are to reap commercial benefits from their inventions and to satisfy industry participants. It may be necessary to reach an agreement on the ownership of potential patents before the start of any project, as it is likely to have financial implications. Rewarding of research that could not be published for commercial reasons may be carried out by the introduction of awards such as the 'git awards' [126] instituted by the collaboration portal, Github. Researchers should also have a common undertaking to respect data protocols, including the need to pay attention to their security and privacy regulations which may differ from jurisdiction to jurisdiction. Thus, a common framework acceptable to all may be useful. Another area that may need addressing is the concept of data sovereignty, which considers that data are subject to the laws and governance structures within the nation it is collected. Although scientific data may be largely exempt from any limitations based on geography, sufficient knowledge of the political environments may be useful.

4.2.6. International funding

Funding is likely to be a major hurdle, and is perhaps best addressed by each member organization supporting their own contribution to the collaborative effort. In addition to annual subscriptions from participating bodies, the umbrella organization may need to be supported by public grants to cover administrative costs. Lobbying for public funding would require much effort by the participating organizations.

5. Summary and a suggested high-level roadmap

In this article, we have made a case for introducing artificial intelligence via digital twins into metal additive manufacturing. We have discussed the need for creating physically validated process models that hold process intelligence, explained the requirement for developing surrogate models through ML, and shown, through an example, how a coordinated global effort can accelerate the pace of research in the field by creating synergies for all participants. We considered the creation of multiscale-multiphysics models and their surrogates and discussed in some depth the significant research opportunities as well as associated hurdles, both technical and non-technical, and offered our thoughts on potential solutions to the identified obstacles.

Numerous complex factors have prevented AM from making significant inroads into the commercial manufacturing sector, despite sizeable investments in research efforts. However, it is our considered view that a greater degree of well-coordinated international collaboration in research, whether informal or formal, can address this. We believe that the introduction of AI can help lift AM, by improving the repeatability of the process and reducing waste, from its present status as a niche, high-end manufacturing technique to an increasingly mainstream method that is more attractive to industry.

Finally, we propose high-level guidance for commencing efforts towards starting conversations that may lead to a meaningful global partnership in metal AM research. This dialog is directed towards the incorporation of AI - through DTs - in industry. The suggested activities are listed in rough chronological order:

1. Approach a society, such as TMS, that holds annual international conferences where international delegates meet, to sponsor initial discussions by appointing an oversight committee.
2. The committee invites a collection of organizations to volunteer to form a core team that takes the lead in steering further discussions.
3. The core team meets (virtually if necessary) to formulate an agenda for broader discussion and feedback. The agenda may include crucial topics, specifically tailored to AM, such as:
   a. Software and hardware challenges in multiscale-multiphysics modeling,
   b.
      i. Standardization.
      ii. Uncertainty quantification.
      iii. Verification and validation.
      iv. Generation of material properties and other input data.

Development of a principled and formal approach (in collaboration with already existing programs) to:
   c. Use of ML in developing surrogate models for real-time queries by DTs.
4. Develop proposals for the above and make them public.
5. Invite expressions of interest to contribute to the topics.
6. Appoint groups with responsibilities commensurate with their strength in topics and track record.

6. Outlook

The global DT market size was valued at USD 3.1 billion in 2020 and is projected to reach USD 48.2 billion by 2026 [127]. Although the projection does not exclusively refer to the scope of the process DT market in metal AM, the underlying technical capabilities and business advantages it provides to AM are unmistakable. DTs when coupled with sensing and control equipment can mitigate defects and improve part quality [9] through real-time closed-loop feedback control, monitor the proper functioning of critical components of printing equipment, and schedule maintenance before failure occurs [128]. Powered by ML algorithms, data, and mechanistic simulations, DTs can guide engineers to minimize trial and error tests, reduce part qualification times, and lower costs [9]. The emerging DT technology can address many of the scientific, technological, and economic challenges faced by metal printing [129]. These and other advantages indicated in this paper can provide unprecedented technical and business advantages of deploying the DTs in metal AM. The continuing improvements in the computational hardware and software and the availability of a technically trained workforce are synergistic factors that are coming together now for enabling such applications.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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