Hybrid digital twins of additive manufacturing combining simulations and machine learning methods

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Abstract. Motivated by the potential for effective substitution of expensive post-production testing, digital twins (DT) are being increasingly implemented within industrial additive manufacturing (AM) settings. DTs aim to combine validated process models with data collected from production to predict the properties and performance of AM parts. Such process DTs have an increasing need for a corresponding accurate materials DT to enable usage within certification and quality control. This paper explores the components of such materials and process DTs, and the typical multiphysics simulation methods and machine learning techniques enabling them.

1. Introduction

The most contemporary formalization of the Digital Twin (DT) concept stems from NASA in 2012, where integrated multi-physics, multi-scale, probabilistic simulations were among the core defining features of a DT together with the data emerging from sensors embedded within systems [1]. Recent reviews [2] have highlighted the DTs of additive manufacturing (AM) processes, their selected characteristics, implementation approaches and chosen success indicators. An example of a DT implementation, that considers the material/microstructure aspects, is the study by Tran et al [3], where integrated computational materials engineering (ICME) methods have been combined with machine learning (ML) techniques to enable anomaly (void) detection in metal AM microstructures in high-throughput dog-bone specimens of 304L and 316L steel, and to evaluate the fatigue and fracture property implications. Similarly, Heo et al [4] have demonstrated a mesoscopic DT, where high-fidelity melt pool dynamics simulations provide the solid-liquid interface information and thermal history data at the micro-meso- length scale to either analytical Lipton-Glicksman-Kurz (LGK) model or numerical phase-field (PF) simulations; which in turn are coupled to the cellular automata (CA) simulations of the meso-scale solidification microstructure via the interface kinetics models. Such a DT has been shown to be able to capture the grain morphology, size and texture emerging during AM with different laser beam shapes, as well as to be deployable in process optimization of the laser beam-shape to avoid typical defects. At an essential level, all such process DTs attempt to emulate how the production process, the material being processed and the product being manufactured relate to the environmental stimuli/conditions, for example, how the temperatures, microstructure and/or stresses vary throughout the object under different conditions.

In this paper, we first highlight the key aspects of the DTs for metal AM processes and AM materials, followed by a brief review of the different simulation models available for establishing the process-structure-properties (PSP) links for AM, and then discuss how different machine learning methods are being applied to aid the establishment of DTs for metal AM. An

implementation of a hybrid DT is showcased, where multiphysics simulations and models derived from characterization/testing are used for predicting the part properties.

2. DT frameworks for AM builds and AM materials

Manufacturing DTs have been implemented at different hierarchical levels, ranging from system of systems (i.e. factory level DTs) to unit level (i.e. process DTs) [5]. The initial motivation behind implementation of these DTs has been stable production under acceptable uncertain/variable conditions and the potential lowering of costs through process optimization. Most studies around AM DTs have thus focused on advancements within either the process modelling aspects (i.e. on the information/model layer) or the sensor-based data acquisition and data analysis aspects (i.e. on the data layer). The granularity of material properties is typically low in most implementations, with continuum/bulk properties (such as Yield stress, Poisson's ratio, S-N curves, etc) based representation being favoured over a description of the inherent heterogeneity in the material microstructure. However, as pointed out by Cogswell et al [6], progressing the technology readiness level (TRL) of manufacturing from TRL6 to TRL9 necessitates a corresponding robust, detailed Materials DT.

From the materials perspective, the information/model layer is responsible for estimating the location specific properties and correspondingly deploys selected models that can translate microstructures into properties (e.g. Hall-Petch equations or micro-mechanical crystal plasticity simulations), while the data layer is responsible for inspecting the microstructural characteristics and measuring the mechanical properties and thereby enabling the update of both the DT as well as the underlying models. Figure 1 highlights the attributes of an AM process DT (i.e the AM build DT) and an AM materials DT (i.e. the AM microstructure DT) and the data exchange required with the corresponding real build and its microstructure. Since the AM process essentially involves melting and re-solidifying metal powders in a repeated process, the process DTs have a primary focus on this aspect. Process DTs setup at the structural-scale have a focus on the temperature fields emerging during the process, the potential defect/void formation during the process, the in-situ heat treatment within the part during the process and the corresponding deformations observed in the part. Process DTs at the scale of the scanning tracks instead focus on the laser-material interaction, the melt dynamics, the plume formation, the spatter formation, and the final solidification of the melt pool. Process DTs at the micro-scale focus on the solidification microstructure and its impact on the melting-solidification process. Most AM build DT implementations attempt to link process DTs at two or more scales, and several different multi-scaling techniques can be found in literature. [2]

Multi-scaling techniques underpin ICME and enable a first-principles based evaluation of the emergent properties as a function of the microstructural characteristics. The DT of the AM

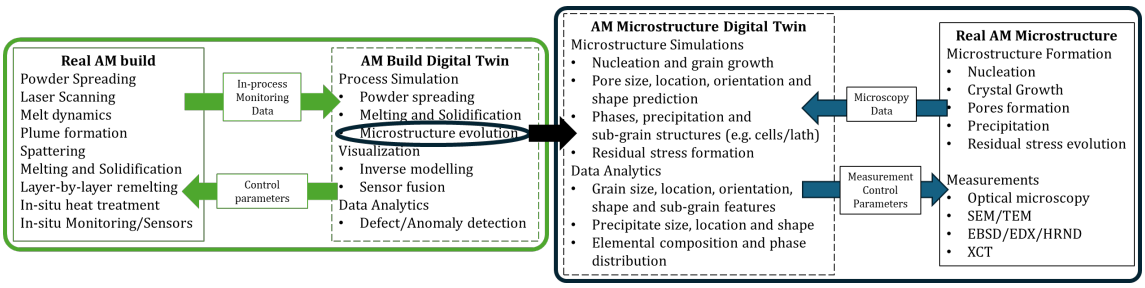


Figure 1. Data exchanged between real and digital twins of AM Builds and AM microstructures. Note: The AM microstructure digital twin is designed to be an intrinsic part of AM Build digital twins

microstructure is typically based on ICME, and forms an intrinsic part of the overall AM build DT. Like the process DTs, the materials/microstructure DTs at different length scales implement different approaches. At the structural scale, the materials/microstructural DT focuses on the polycrystalline structure, the residual macro-stresses and the consequent mechanical properties. At the meso-microscale, the focus shifts to nucleation and crystal growth during solidification, pore formation, recrystallization, thermo-mechanically induced phase transitions. At the micro-nano scale, phenomena such as precipitation come into focus together with grain boundary migration, elemental transport, corresponding interface kinetics as well as inter/intra-grain micro-stresses. ICME models capable of capturing these phenomena occurring at different length scales are typically calibrated and validated via a range of characterisation methods (such as XCT, EBSD, EDX, SEM, TEM, high resolution neutron diffraction(HRND), etc) that create the datasets necessary for establishing material DTs. Since the modality of microstructural data can be varied at the different length scales, establishing a systematic framework for describing the material data is a challenge. Strategies such as the n-point spatial correlations framework [7] or the MKS framework [8] attempt such a unified description across atomic to microscales, and result in a set of large number of features that can be selectively used by models at different length scales. Consequently, assuming accurate microstructure simulations are feasible, the AM microstructure DTs can potentially provide the parametric PSP links needed for establishing AM build DTs.

3. Simulation and testing based approach for AM Process-Structure-Property links

As the features of interest for AM DTs occur at different length scales, the numerical simulations of AM processes rely on coupling strategies that operate at these length-scales and accordingly have varied fidelity levels [10]. Figure 2 highlights a multi-scale approach for establishing the PSP link for Ti6Al4V parts manufactured by metal AM. Specimens for tensile testing (see figure 2(a)), as well as coupons for fatigue and crack growth analysis, were designed to capture the orientation, size and location effects for AM parts. Mechanical testing (see figure 2(b)) were performed for as-built, machined/polished as well as heat-treated parts. To correlate the mechanical tests to the microstructural features, the parts were analysed by X-CT methods (for internal voids), optical microscopy techniques (for surface characteristics) and SEM imaging (for grain and sub-grain features statistics) (see figure 2(c) and 2(d)). The approach of capturing detailed images of internal microstructures of parts, which are subsequently meshed and used in advanced non-linear finite element (FE) load analysis to predict the mechanical performance of parts, has been demonstrated and validated with in-situ Digital Volume Correlation (DVC) analysis[11].

Establishing a causal link for the PSP begins with establishing models for predicting the temperature fields, the solidification microstructures and the micro-mechanical behaviour of the resulting polycrystalline microstructure [12-14]. A key enabler is the prediction of thermal fields during the AM processes at the right level of accuracy (see figure 2(e) and (f)). Macro-scale simulations become relevant when the trends in the thermal history have greater impact compared to the precise estimation of peak temperature values. Often implemented using FE tools, the macro-scale simulations are fast and aim at predicting the temperature distributions, the average phase fractions, the global residual stresses as well as the eventual deflection when a part is manufactured and post-processed [15]. The microstructure is often considered as a continuum for these models, while retaining the location-specific inhomogeneity information (e.g. the local phase fractions based on thermal history) and the temperature dependence of mechanical properties. For more accurate DT representations, however, micro-meso scale simulations become relevant. The finite volume/FE based CFD techniques or Lattice Boltzmann

methods can simulate the melt pool's fluid dynamics, the free surface and interface conditions as well as the consequent flow-induced defects such as dross and porosity formation [16-17]. The predicted temperature field is a necessary input for the microstructural models at the micro-meso scale, which are normally implemented using either CA (figure 2(i)) or kinetic Monte Carlo (MC) techniques [18-20]. Typical grain structures formation mechanisms, including nucleation and epitaxial growth, bulk nucleation, competitive growth, and columnar-to-equiaxed transition are captured by these microstructural models [15], the material parameters for which are evaluated using CALPHAD (Calculation of Phase Diagrams) based methods. Approaches such as the CA-FE couple the macro-scale thermal predictions to meso-scale microstructures in a computationally efficient manner, while coupling meso-scale thermo-fluid models, MC and crystal plasticity finite element methods (CPFEM) [13, 21-22] allows a more accurate PSP link prediction. Figure 2(g)

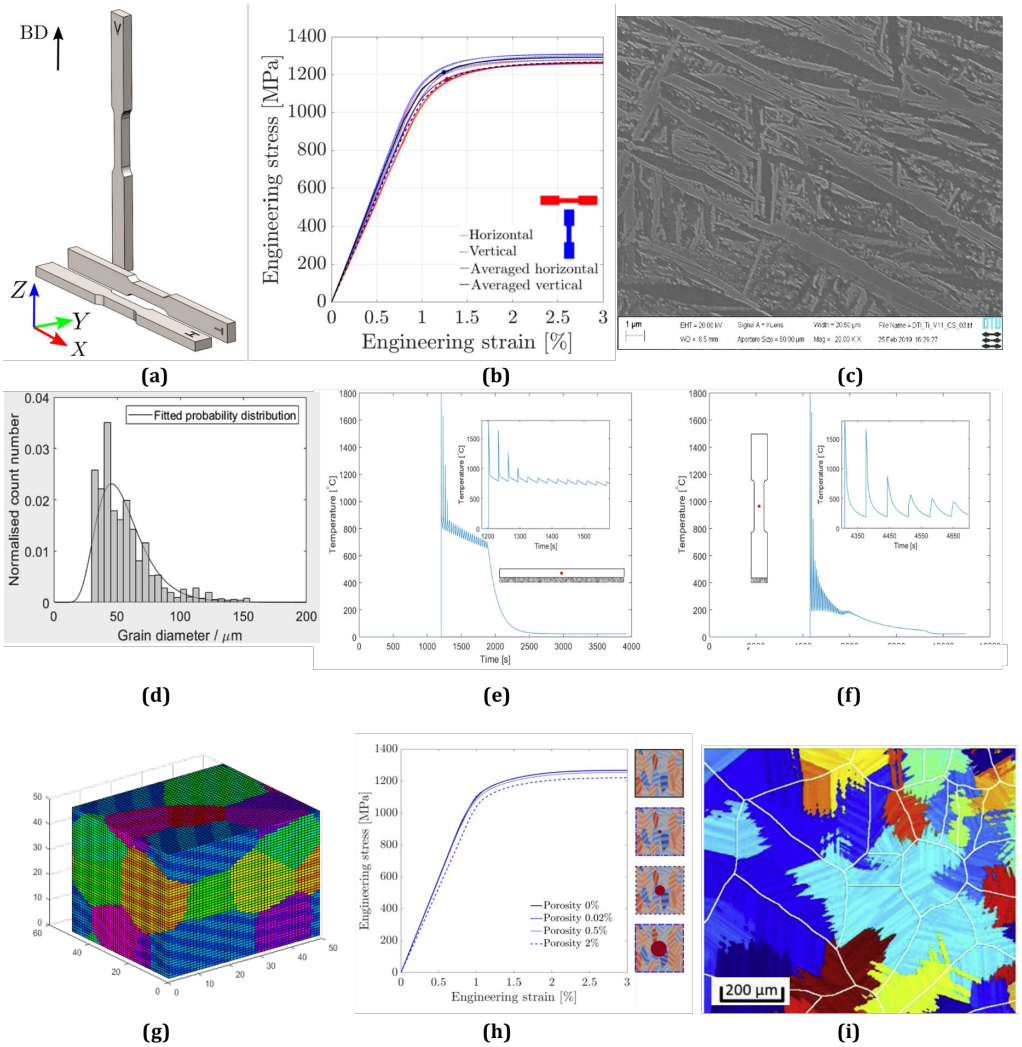


Figure 2. Process-structure-properties links for AM Ti6Al4V (a) Test specimens designed to capture orientation effects [12], (b) Experimental tensile tests for mechanical properties [13], (c) SEM image of vertical specimen (scale is 1um) [14], (d) estimated as-built grain size statistics from microscopy and image analysis [15], (e) and (f) Simulated thermal history at center of horizontal and vertical dogbone specimens respectively [14], (g) periodic RVE generated using microscopy data showing secondary lath features, (g) CPFEM simulated impact of porosities on the mechanical properties of Ti6Al4V[12], & (i) predicted microstructure for above β-transus heat treatment by CA [15].

and (h) highlight such a micro-scale simulation implementation where predicted representative microstructures from the AM process were used to predict the mechanical behaviour of the material in presence of different levels of porosity.

As the solidification microstructures emerging from AM are typically non-equilibrium and metastable, the subsequent thermal cycling during the production of the part induces phenomena such as recyrstallization, phase transition, precipitation, etc. Capturing such aspects, especially at the sub-grain level, necessitates nano-micro scale models – such as those based on PF simulations [23]. The applicability of the PF method is contingent on the availability of the thermodynamic descriptions of the material systems, and while Molecular Dynamics (MD) simulation workflows exist at the nano-scale for prediction of these thermodynamics parameters for the micro-scale PF models, currently the MD models cannot adequately take into account the actual processing conditions. Consequently, most material DTs for AM typically span from the structural-scale to the micro-scale, with the noted exception of DTs for AM of high-entropy alloys [24].

5. Machine learning for predictive modelling and microstructure analysis

Validated simulation workflows allow for digitally establishing the PSP relationships for AM from a first-principles approach. However, implementation of these multi-scale multi-physics models within a real-time DT scenario is currently computationally prohibitive. As an alternative approach, the real data from experiments can be used to achieve a reduction of the dimensionality of the models, through techniques such as Proper Orthogonal Decomposition, Gaussian process regression, Polynomial Chaos Expansion or neural networks. Recent studies have demonstrated the potential for using such machine learning (ML) methods to predict occurrence of local defects like porosity and micro-cracks [25-26], as well as for predicting melt pool dimensions during the AM process based on sensor data [27-28]. The AM dataset is multi-modal and can contain data related to the sets of AM process parameters used, the in-situ measured process signatures during AM, the database of material behaviour data for the processed alloys, and the characterization and testing data measured during post-process analysis. Combining such diverse data into a coherent dataset is challenging, and only a few high-quality full datasets exist for AM materials within open scientific literature e.g. the AMBench dataset from NIST for the most commonly used AM materials (316L, Ti6Al4V, IN625, IN718). Similarly various material property databases, containing material data ranging from elastic, thermal, electro-chemical properties to DFT-based properties and crystal structure information, are becoming available e.g. AFLOW, Open Quantum materials Database, Polyinfo Polymer Database, and Crystallography Open Database.

ML techniques become particularly relevant when the static information from the AM databases need to be combined with the massive amounts of dynamic process signature data being captured via advanced in-situ monitoring methods [29] . It is increasingly common for industrial AM machines to contain a range of in-situ monitoring equipment, ranging from stereo vision optical cameras, thermal cameras, co-axial pyrometers, acoustic sensors, eddy current based sensors, flash interferometry based thermography systems, etc. These sensor data must form the primary basis for part qualification and certification in the future, in lieu of testing and characterization of each AM build. Therefore, a need exists for high robustness of the decision making models that evaluate the part quality and high quality for the validation datasets upon which these models are trained. Supervised ML techniques such as Naive Bayes classifier models, k-Nearest-Neighbour method, Decision Trees, Kernel methods, Support Vector Machines, and Artificial Neural Networks have been investigated in recent years for establishing such anomaly detection and digital part quality evaluation setups. Review studies by Durodola [30] and Che et

al [31] have discussed the application of ML to the problems of material discovery/selection, alloy development, in-situ process parameter control as well as parameter optimization. In the reviewed studies, ML techniques (see figure 3(a)) have been combined with different process simulations to establish the property prediction feature suitable for DT implementations. A review of studies establishing the PTSP linkages (i.e. process-thermal, process-structure, process-property, thermal-structure, etc), and the corresponding model inputs and outputs for each category can be found in [19], focusing on SS316L, Ti6Al4V, Inconel 718/625, SS 17-4PH and AlSi10Mg. Further, convolution neural networks (CNN) based methods are being increasingly applied within material DTs of AM (e.g. for high-throughput image segmentation [32] and microstructure classification, see figure 3(b)) since these techniques can directly utilize high quality microscopy data and imaging/tomography data (including EBSD, EDX and HRND data) from AM builds. More extensive recent reviews of machine learning methods application to AM [9], microscopy [32] and ICME [33] can be found in literature for gaining further insights.

6. Hybrid DTs

Validated DTs are often developed as "fit-for-purpose" solutions rather than a generic representation of the real AM process. The efficiency and the scope of application of these DTs are thus highly dependent on the quality of the underlying validation datasets, the chosen fidelity and complexity of the models utilizing the data, the quality of the in-situ senor measurements that provide the real process information, as well as the execution strategy/infrastructure supporting the deployment of such DTs (e.g. on-machine IoT OR edge computing OR cloud computing implementation). Multiphysics simulation-based approaches and ML enabled data-based approaches to DTs are both viable pathways for industrial implementation, yet currently suffer from inherent challenges. On the data-driven DT side, typically, the validation/training datasets collected from a typical data source are generated via a single experimental campaign, and thus is only capable of providing incomplete and uncertain insights into the complete set of physical phenomena (e.g, when the training dataset is generated through experiments with a single batch of powder, it cannot account for influence of batch-to-batch variability in powder characteristics). Similarly, the simulation-driven DTs are only capable of providing prediction of the material

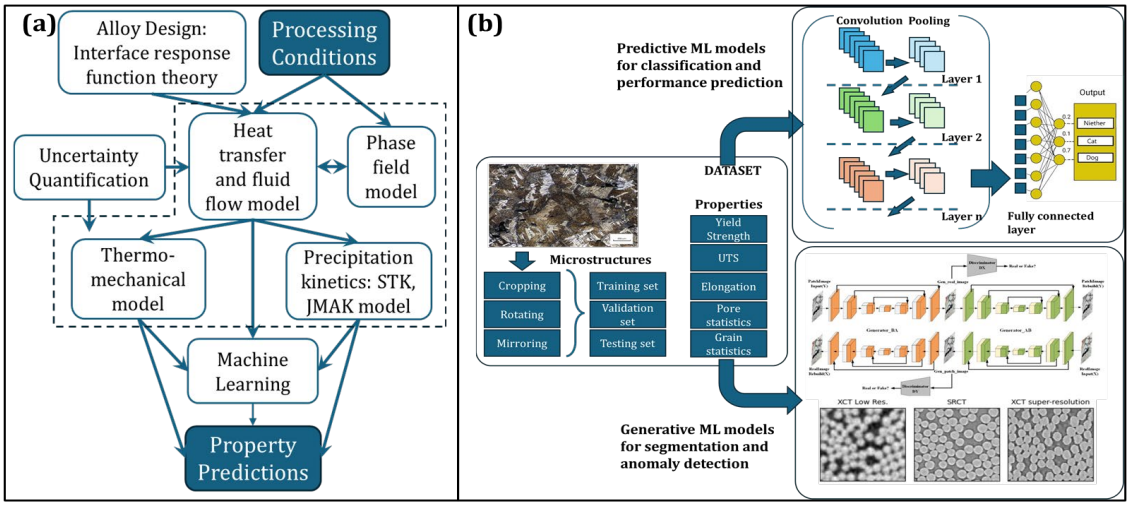


Figure 3. Application of machine learning methods for establishing process-structure-properties links through (a) simulation-driven workflows, and (b) data-driven workflows

behaviour based on user-specified multiphysics models i.e. they cannot account for situations where either the underlying modelling assumptions are invalidated as well as where the dominant governing physics are not adequately defined in the model (e.g. a classical thermo-mechanical model based on bilinear plasticity formulations cannot account for the changes in the local yield strength and Youngs modulus due to dislocation density evolution).

Hybrid DT implementation approaches identify these limitations and aim to utilize a combination of both techniques where relevant. For instance, rigorous multi-physics simulations are utilized for property prediction when accurate measurements of the actual environmental stimuli are available, while data-based models are preferred when higher levels of uncertainty exist for either the applied process setting and/or the measured environmental stimuli. Here, the needed accuracy level for predictions and the available computation time determine the selection of the relevant process models and the type of data (modality, frequency, etc.) used for predictions. Thus, instead of being constituted of a single model and dataset, hybrid DTs are characterised by a multitude of models of different fidelity, complexity, physics and prediction accuracy/uncertainty. Hybrid DTs also contain multiple validated sub-datasets with different characteristics (i.e. granularity, resolution, quantified uncertainty, etc), that can accurately capture the influence of a sub-set of process parameters and environmental stimuli. A key feature of hybrid DTs then constitutes the decision-making algorithms that can identify and deploy the appropriate model(s), as well as apply the corresponding appropriate data assimilation/filtering methods (e.g. when the selected thermal model can predict temperatures with an accuracy +/- 10^{o}C with an output resolution of 0.1Hz, the incoming measurement data from other local sensors would also be aggregated/filtered to have the same resolution).

7. Future Outlook

As the digitisation of the design-manufacture-test/characterize work-flow progresses, a multitude of DTs corresponding to the AM process, the production equipment, the environmental (factory) settings, the raw materials and the product will emerge. Specifically, developments in AM microstructural DTs are expected, with hybrid DT implementations finding increased adoption as the same framework could be used for the different stages of the product life cycle.

Most AM simulation studies currently achieve multi-scaling through constitutive modelling, and multiphysics integration by sequential coupling of independent simulations (e.g. by parameter passing). As the computing power continues to increase exponentially (like over the last decades), direct thermo-microstructural-mechanical simulations of large domains (across three orders of magnitude in the length scale) will become feasible on individual workstations, potentially paving the way for rigorous future studies implementing multi-scale multiphysics simulations for AM. Advanced multi-scaling methods will still remain relevant and will continue to be developed as we slowly approach the post-Moore era of computing power.

Advancements in ML methods is further projected to increase the viability of AM DTs. With increased access to cloud computing and dedicated algorithms optimized for supervised/deep learning, a rapid expansion of fundamental material databases is expected. In parallel, high-speed data acquisition equipment and data filtering algorithms continue to be developed, enabling reinforcement/transfer learning of existing AM material DTs to other materials in the same family (i.e. with similar behaviour). Together with high-throughput testing protocols being developed for AM, it implies a rapid expansion can be expected for the datasets that are available for establishing the P-S-P relationships in different AM materials.

Progress in the domain of decision-making algorithms and model deployment, along with the increased availability of on-demand computing, will allow true in-parallel or co-simulations of the process, microstructure and expected properties along with actual AM process. Thus, in future, validated AM microstructural DTs will become an intrinsic part of AM Build DTs, where predictive models of microstructures can modify the AM process in a feedback/feedforward manner.

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