Intelligent Digital Twins can Accelerate Scientific Discovery and Control Complex Multi-Physics Processes

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Abstract

The emerging area of Intelligent Digital Twins (IDTs) offers great potential as a new paradigm for accelerating scientific discovery, while also offering state-of-the-art functionality in controlling complex physical processes. We investigate this concept for the case of an Intelligent Digital Twin of metal additive manufacturing (AM). Metal AM is an excellent choice for utilising of an IDT due to the process being an inherently complex multi-physics one, with key elements including granular powder flow, laser melting and material solidification. This complexity means that computational simulations are extremely costly and obtaining high quality experimental data extremely difficult, so optimal exploration of the parameter space using all available information on the current uncertainty in the region of interest is highly desirable. Our Intelligent Digital Twin for this process includes a complete description of the target geometry of the object being printed and a set of data-driven and computational models for the different physical processes occurring in the system. The data-driven models consist of a set of Gaussian Processes (GP) that can be trained using combinations of real world sensor data and outputs from computational simulations. We illustrate the utility of our IDT by determining optimal input print parameters and obtaining Pareto fronts between competing priorities such as surface roughness and print time. We also demonstrate the potential of the IDT as an intelligent control system to respond to errors during the print process and dynamically improve final print quality.

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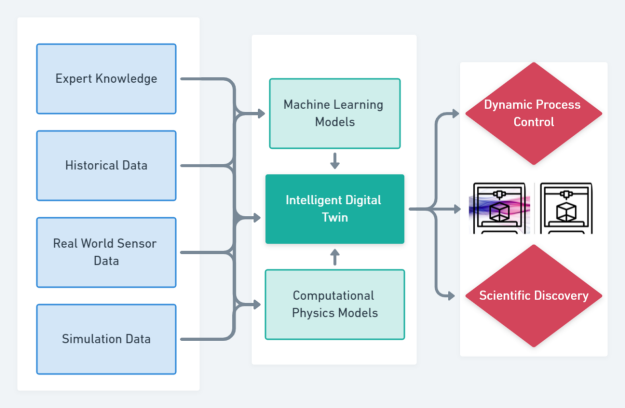

Figure 1. Schematic Diagram of the core elements of the Intelligent Digital Twin.

1. Introduction

The term Digital Twin was originally coined by NASA in 2010 as an "integrated multi-physics, multi-scale, probabilistic simulation of a vehicle or system that uses the best available physical models, sensor updates, fleet history, etc., to mirror the life of its flying twin" (Piascik et al., 2010; Shafto et al., 2010). Digital twins went on to become the primary framework used by NASA and others for virtual testing of spacecraft and prediction of future failure events (Tuegel et al., 2011; Glaessgen & Stargel, 2012) and also became ubiquitous in many other diverse application areas including building management, smart cities, healthcare, logistics and manufacturing (Fuller et al., 2020).

More recently the concept of hierarchies of Digital Twins has emerged, with the most sophisticated of these referred to as an "Intelligent Digital Twin" (IDT) (Phua et al., 2022). Such an IDT has all the characteristics of lower level Digital Twins in terms of their ability to model, sense and interface to the physically twined object or process, but adds an additional intelligence to reason about current system state and autonomously tailor and optimise parameters in the physical twin (See Figure 1). However, one hitherto not well explored use case is the application of such an intelligent digital twin as a key component in the scientific discovery

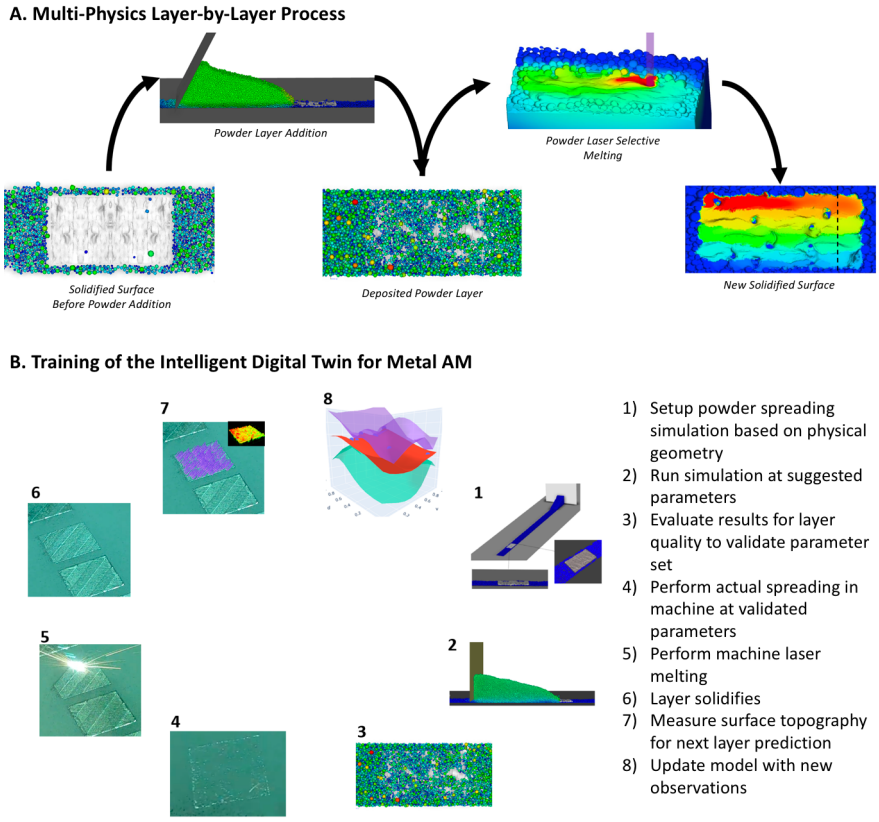

Figure 2. (Top, **A**) Key elements of the multi-physics process that occur during the addition of a single layer of material in selective laser melting additive manufacturing. A powder layer is added to the existing surface of solidified material and selective melted in to the required layer geometry and then the process is repeated. (Bottom, **B**) Illustration of keys process steps for data acquisition for training of the Intelligent Digital Twin using a combination of computationally generated and real world sensor data.

process. This kind of framework can offer many significant benefits. Sensorisation technologies have become much more ubiquitous and affordable, allowing for the detailed measurement of a wide variety of complex system states, while in parallel advances in available computational power and a desire to model and understand ever more detailed physical processes have led to an explosion in interest in the study and optimisation of complex multi-physics systems. The Intelligent Digital Twin has the potential to be at the heart of this process, with applications including utilising uncertainty about current model state to control data acquisition through to the integration of faster-than-real-time surrogate models that can be used at runtime to optimise and control a complex physical processes. In this paper, we will demonstrate the utility of this paradigm for the case of a complex multi-physics example from metal additive manufacturing (AM).

2. An Intelligent Digital Twin for Metal Additive Manufacturing

We will consider the case of metal additive manufacturing (or more colloquially referred to as metal 3D printing) and the application of an Intelligent Digital Twin informed from a set multi-physics models and realtime sensor data. Metal AM shows incredible promise for revolutionising the manufacture of bespoke parts in diverse areas including aerospace, biomedical and automotive applications (Samuel et al., 2018; Lowther et al., 2019). However, many challenges remain in unlocking its full potential due to the need to understand the complex multi-physics nature of the problem, and the very large computational power required to simulate such processes (Phua et al., 2022). Two key challenges are understanding and optimising the input material behaviour (Erps et al., 2021), the parameters utilised during the printing process (Deneault et al., 2021) - including print orientation (Goguelin et al., 2021), lattice geometry (Hertlein et al., 2020) and strut design (Gongora et al., 2020).

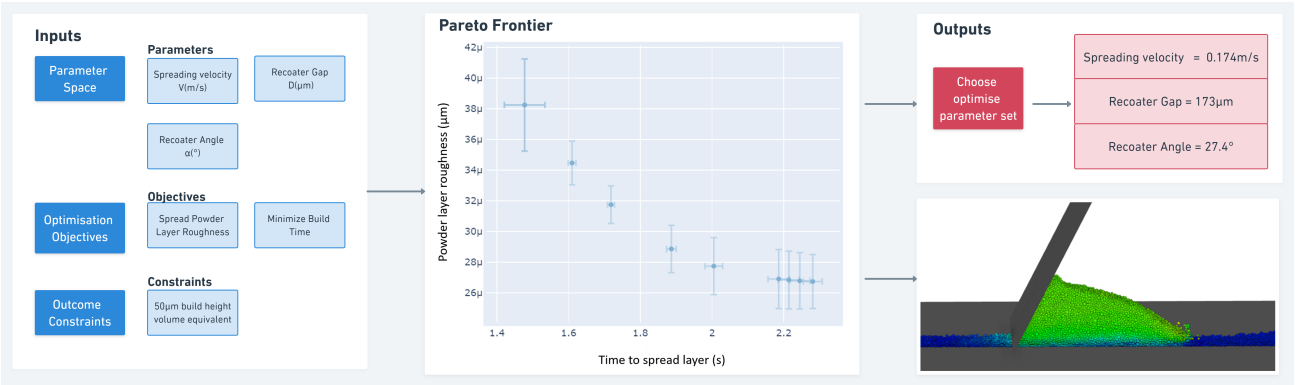

Figure 3. Gaussian Process Optimisation of the time taken to spread the powder layer and its resulting roughness, subject to a constraint requirement of achieving an addition of a $50\mu m$ height volume equivalent of powder. The Pareto Frontier showing the trade-off between powder layer roughness and the time taken to spread the powder is shown in the center.

We will use metal AM as a use case to illustrate how the intelligent digital twin (IDT) can be utilised by:

- Optimally sampling the parameter space in regions of interest utilising a minimal number of expensive computational simulations and real world measurements. The use of Bayesian approaches and a continual quantification of the IDT model uncertainty are critical elements to this.
- Training surrogates that can then be used for faster than real time predictions.
- Controlling the physical twin process by maintaining the accuracy of the IDT state through continual sensor inputs, and autonomously modifying process parameters to correct for any out of specification behaviour.

Figure 2 shows the key elements of the most commonly employed selective laser melting metal AM process. The process works by iteratively adding layers of a metal powder (e.g. titanium) on to the existing print surface, melting the powder with a laser in the layer geometry required, allowing the material to solidify and then lowering the stage and repeating the process. Metal AM consists of several highly complex physical material processes, including elements of granular powder flow during the recoating stage, heat transfer from the laser and through the material, and state change via melting and subsequent resolidification into a complex microstructure that can strongly influence final part strength and behaviour (Wycisk et al., 2014; Gong et al., 2015).

Our Intelligent Digital Twin for this process includes a complete description of the target geometry of the object being printed and a set of data-driven and computational models for the different physical processes occurring in the system. The computational models include a DEM based powder flow model (Phua et al., 2021), a volume of fluid solution to the melting and resolidifcation (Cook & Murphy, 2020) which can then be fed in to a microstructure model to determine final part material composition and behaviour (Cummins et al., 2021). The data-driven models consist of a set of Bayesian Models consisting of Gaussian Processes (GPs) that have can trained using combinations of experimental and computationally generated data. GP models have been successfully applied to several additive manufacturing systems and shown to be able to create accurate process maps and surrogate models for expensive laser melting simulations (Tapia et al., 2016; 2018; Kamath & Fan, 2018), and printability maps for metal AM (Johnson et al., 2019).

For the Gaussian Process models contained within our IDT, we use a Matern 5/2 kernel function chosen for its flexibility and smoothness (Rasmussen & Williams, 2006; Balandat et al., 2020) and a sampling strategy using an initial Sobol quasi-random generator to initialise points within the parameter space, followed by an Expected Improvement (EI) acquisition function. The GP model is then used by the IDT to choose the next query point based on maximal potential improvement of the target objective. Our sampling strategy can explore a number of new trials in parallel where possible to accelerate the optimisation process, at the trade-off of less frequent updates to the model.

3. Optimisation of Process Parameters

Critical to the entire AM process is the uniform application of smooth layers of powder and their highly localised melting and solidification in to a precise surface for the next layer addition. A very large amount of research goes in to finding the optimal input feed materials and optimal process parameters for use in metal AM (Sames et al., 2016). The

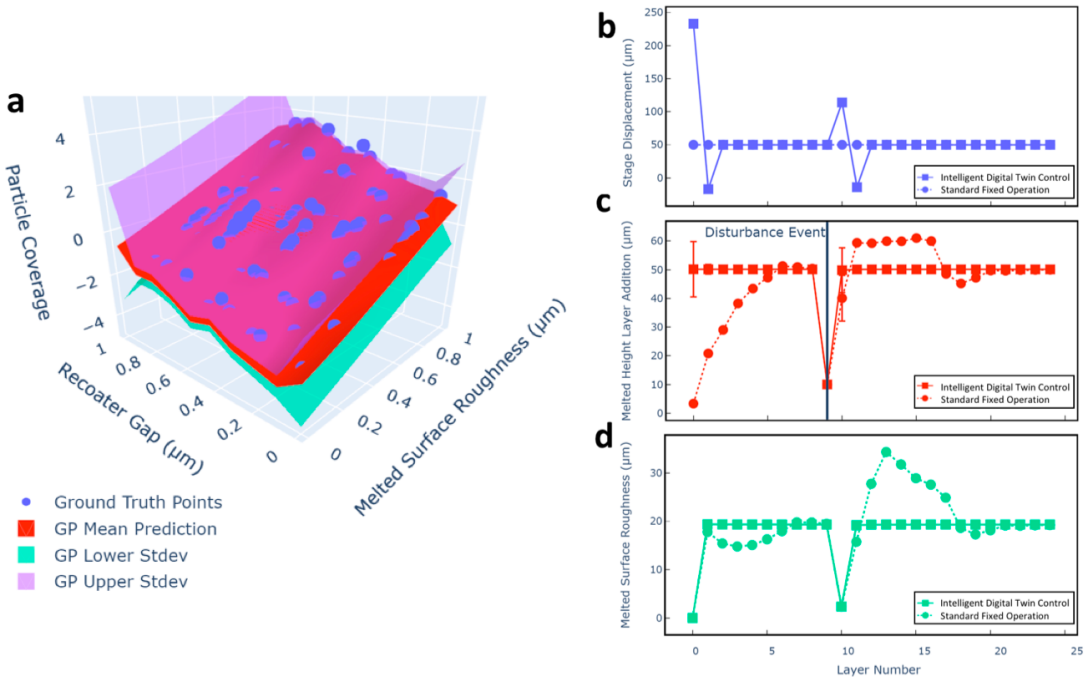

Figure 4. (a) Gaussian Process Model trained to predict how the height of the added material layer varies with the recoater gap and the melted substrate surface roughness. (b,c,d) Example of a disturbance event during the print process at layer 10 where only 20% of the required material is deposited. Note the subsequent difference in the time required for the system to reequilibrate for the standard fixed operation case vs. when under the control of the Intelligent Digital Twin.

IDT can be extremely useful in optimising these parameters. Figure 3 shows the Pareto front for optimising the roughness and spreading time of the layer, which is a typical trade-off that must be made when tuning the powder-spreading process. Here we have constrained the volume deposited on to the surface to match the stable state deposition requirement that ensures consistent volume additions equivalent to a 50µm build height. This information can then be used to find the machine parameters that are sufficient to keep the process within the desired tolerances, while minimising the build time.

4. Real-time Process Control

Current AM systems generally utilise an established set of optimal process parameters that do not dynamically adjust during the build process. However, the build process in Metal AM inherently relies on consistent layer additions to print intricate parts with fine tolerances and detail. Paramount to this process is ensuring consistent and even additions of build material in each layer. For most AM processes, this poses a significant challenge, as printers often employ fixed print parameters throughout the duration of a build, which only converge to steady-state after several layers (Mindt et al., 2016). Moreover, defects and disturbances in the printing process are commonplace and inject transient variability (Scime & Beuth, 2019). This can lead to variations in the distance between the recoater and the current solidifed layer within the printer, which can cause out of specification behaviour such that the print process can fail entirely.

We demonstrate how we can tackle the problem of correcting for a single bad deposition layer where a below specification volume of material has been added with a corresponding out of spec surface rough surface being created. To control the inter-layer variability we employ Bayesian Optimisation to train a GP surrogate model that can be used to dynamically control the print parameters to ensure consistent layer quality. We first train a set of GP models to determine optimal powder spreading parameters on a set of 12 unique surface roughness geometries that span those commonly found in real world print cases, and in this way determine a high dimensional relationship between the melted surface roughness and the required recoater gap to achieve consistent layer additions. A key outcome of this study is the accumulation of a sufficient training data set that can then be used to train a single GP surrogate model that covers the entire domain (Figure 4a). This surrogate model can then be used in real time during the build process, with

the IDT reading in sensor data and intermittently querying the surrogate model for optimal parameters for real-time control and enhancement of the printing process. Using this surrogate, we can inform the printer between layers what the correct stage displacement ought to be. In contrast, printers today naively employ a fixed stage displacement at each layer, which produces instability in layer additions that only stabilise after 7-10 layers.

Figure 4b-d demonstrates the ability of the intelligent digital twin to control for a defect event during the print process. Here we simulate the case of our IDT controlling a variable stage displacement at each iteration - compared to most AM machines today that use a standard fixed stage displacement. Our results compare the performance between the two systems over 25 layers of printing when a defect is introduced at layer 10. We simulate a typical recoating defect by decreasing the powder coverage to 20% of its nominal value. When the defect occurs, our IDT detects this and responds by sending the printer an updated set of machine parameters (with a corrected stage displacement) to return the system to equilibrium within just two layers. In contrast, the baseline system takes more than 10 layers to return to equilibrium and steady-state layer additions after the system disturbance. Our results highlight how small print disturbance can lead to instabilities across multiple layers in 3D printed parts. More critically, our results demonstrate the utility of a IDT system for mitigating such defects and achieving consistent print quality in each layer.

5. Conclusions

We have demonstrated the potential benefits of the new emerging paradigm of Intelligent Digital Twins as a tool for accelerating scientific discovery and intelligent control of complex multi-physics systems. The IDT can combine all available historical information about a process, integrating computational models based on the underlying physics/chemistry/biology and data-driven models trained using both computational and real world sensor data. Through the integration of Bayesian Optimisation techniques, the IDT can fulfill a key need in providing an optimal way to explore the available parameter space and optimise the input parameters for the best process performance. The integration of faster than real time surrogate models into the IDT also opens up exciting new applications for their use at in predicting future out-of-spec behaviour for a process and enabling corrective action to be taken. For the case of metal AM, this opens up particularly exciting new possibilities in the integrated design of new materials and processes that can utilise IDTs to dynamically maintain specification compliance during the print process.

Acknowledgements

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