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 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 is 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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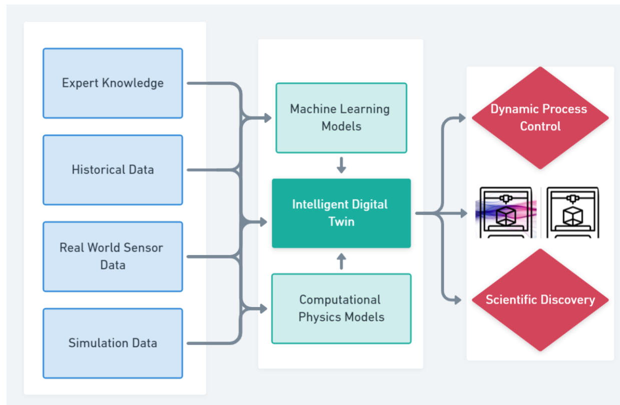

Figure 1. Schematic diagram of the core elements of the Intelligent Digital Twin.

1. Introduction

The term Digital Twin was originally defined 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 rapidly became 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., 2022b). 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 machine 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

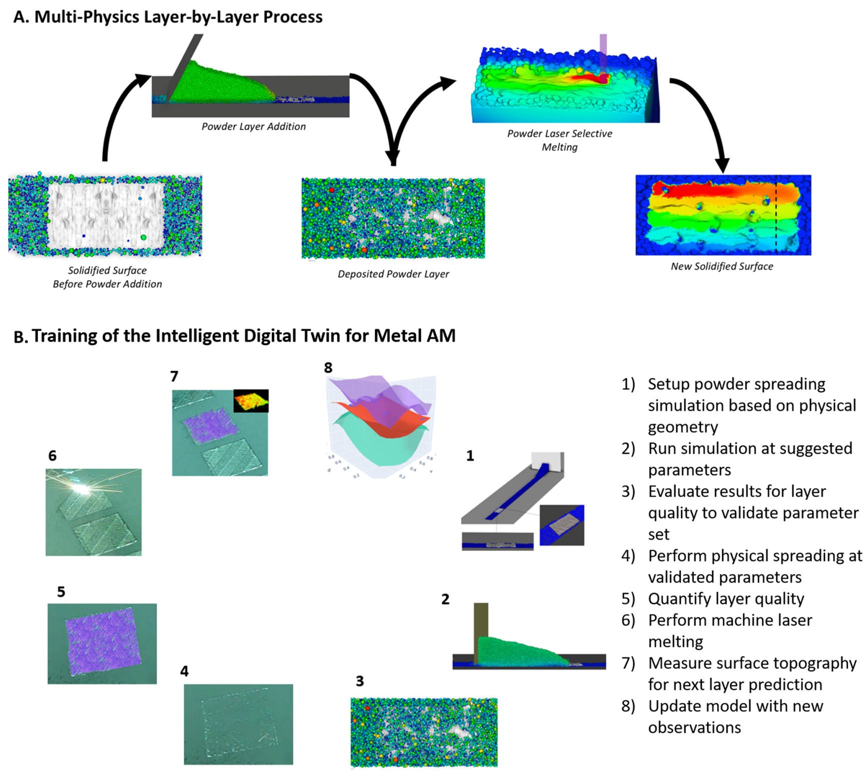

Figure 2. (Top, **A**) Key elements of the multi-physics process that occur during the addition of a single layer of material in selective laser melting additive manufacturing. A powder layer is added to the existing surface of solidified material and selective melted in to the required layer geometry 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.

digital twin as a key component in the scientific discovery 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 states 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 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., 2022a). Two key challenges are understanding and optimising the input material behaviour (Erps et al., 2021) and 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).

We will employ metal AM as a use case to illustrate how

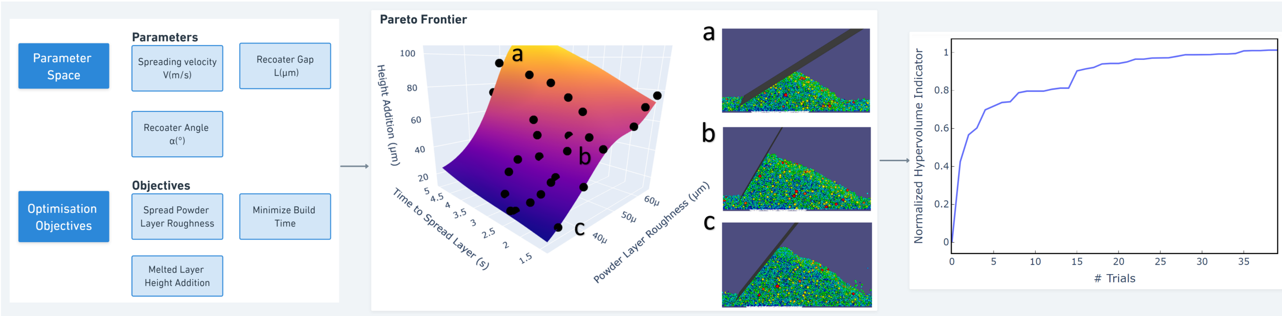

Figure 3. Multi-Objective Bayesian Optimisation of powder recoating for process discovery. The Pareto Frontier showing the trade-off between powder layer roughness, the time taken to spread the powder and the material height addition is shown in the center, together with images of newly revealed operational strategies. The hyper-volume indicator is shown on the right.

the intelligent digital twin (IDT) can be utilised by:

- Optimally sampling the parameter space in regions of interest using 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) and a volume of fluid solution to the melting and resolidifcation (Cook & Murphy, 2020), which can then be fed into 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 have been 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 or qNEHVI (Daulton et al., 2021) for multi-objective optimisation. The GP model is then used by the IDT to choose the next query point based on the 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.

3. Scientific Discovery using Bayesian Optimisation

Critical to the entire AM process is the uniform application of smooth layers of powder and their selective melting and solidification into precise surfaces for the next layer addition. A large amount of research goes into finding the optimal input feed materials and optimal process parameters for use in metal AM (Sames et al., 2016). The IDT can be extremely useful in optimising these parameters by performing virtual experimentation.

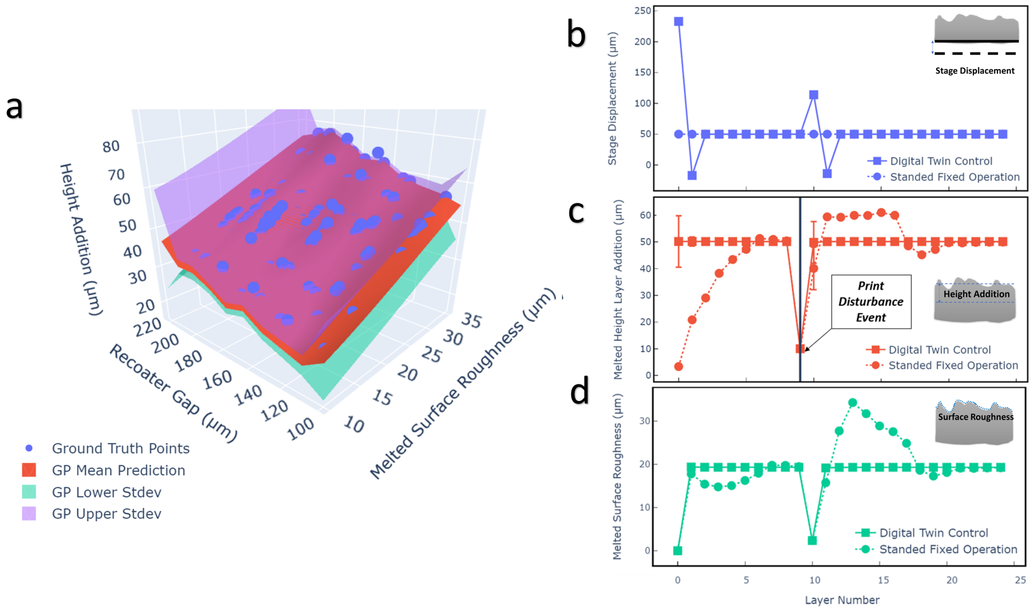

Figure 4. (a) Gaussian Process Model trained to predict how the height of the added material layer varies with the recoater gap and the melted substrate surface roughness. (b,c,d) Example of a disturbance event during the print process at layer 10 where only 20% of the required material is deposited.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

An adaptive experimentation pipeline enables an efficient scientific discovery process for new printing strategies and techniques. Figure 3 shows our implementation using multi-objective optimisation, which produces a Pareto front by configuring and running new virtual experiments to efficiently explore the parameter space. The Pareto front optimises the addition of material layer height, the roughness of the layer, and the operation time, which are typical trade-offs that must be made when tuning the powder-spreading process. The optimisation process reveals new process strategies for the printer's operation, which aids in the discovery of new mechanistic effects.

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 metal AM build process 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 optimal stage displacement should 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 printing 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 disturbances can lead to instabilities across multiple layers in 3D printed parts. More critically, our results demonstrate the utility of an 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 fulfil 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 as a tool for 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

References

Balandat, M., Karrer, B., Jiang, D. R., Daulton, S., Letham, B., Wilson, A. G., and Bakshy, E. BoTorch: A framework for efficient monte-carlo bayesian optimization. In *Advances in Neural Information Processing Systems 33*, 2020.

Cook, P. S. and Murphy, A. B. Simulation of melt pool behaviour during additive manufacturing: Underlying physics and progress. *Additive Manufacturing*, 31:100909, January 2020. ISSN 2214-8604. doi: 10.1016/j.addma.2019.100909.

Cummins, S., Cleary, P. W., Delaney, G., Phua, A., Sinnott, M., Gunasegaram, D., and Davies, C. A Coupled DEM/SPH Computational Model to Simulate Microstructure Evolution in Ti-6Al-4V Laser Powder Bed Fusion Processes. *Metals*, 11(6):858, June 2021. doi: 10.3390/met11060858.

Daulton, S., Balandat, M., and Bakshy, E. Parallel Bayesian Optimization of Multiple Noisy Objectives with Expected Hypervolume Improvement. In *Advances in Neural Information Processing Systems*, volume 34, pp. 2187–2200. Curran Associates, Inc., 2021.

Deneault, J. R., Chang, J., Myung, J., Hooper, D., Armstrong, A., Pitt, M., and Maruyama, B. Toward autonomous additive manufacturing: Bayesian optimization on a 3D printer. *MRS Bulletin*, 46(7):566–575, July 2021. ISSN 1938-1425. doi: 10.1557/s43577-021-00051-1.

Erps, T., Foshey, M., Luković, M. K., Shou, W., Goetzke, H. H., Dietsch, H., Stoll, K., von Vacano, B., and Matusik, W. Accelerated discovery of 3D printing materials using data-driven multiobjective optimization. *Science Advances*, 7(42):eabf7435, 2021. doi: 10.1126/sciadv.abf7435.

Fuller, A., Fan, Z., Day, C., and Barlow, C. Digital Twin: Enabling Technologies, Challenges and Open Research. *IEEE Access*, 8:108952–108971, 2020. ISSN 2169-3536. doi: 10.1109/ACCESS.2020.2998358.

Glaessgen, E. and Stargel, D. The Digital Twin Paradigm for Future NASA and U.S. Air Force Vehicles. In *53rd AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference*, Honolulu, Hawaii, April 2012. American Institute of Aeronautics and Astronautics. ISBN 978-1-60086-937-2. doi: 10.2514/6.2012-1818.

Goguelin, S., Dhokia, V., and Flynn, J. M. Bayesian optimisation of part orientation in additive manufacturing. *International Journal of Computer Integrated Manufacturing*, 0(0):1–22, September 2021. ISSN 0951-192X. doi: 10.1080/0951192X.2021.1972466.

Gong, H., Rafi, K., Gu, H., Janaki Ram, G. D., Starr, T., and Stucker, B. Influence of defects on mechanical properties of Ti–6Al–4V components produced by selective laser melting and electron beam melting. *Materials & Design*, 86:545–554, December 2015. ISSN 0264-1275. doi: 10.1016/j.matdes.2015.07.147.

Gongora, A. E., Xu, B., Perry, W., Okoye, C., Riley, P., Reyes, K. G., Morgan, E. F., and Brown, K. A. A Bayesian experimental autonomous researcher for mechanical design. *Science Advances*, 6(15):eaaz1708, 2020. doi: 10.1126/sciadv.aaz1708.

Hertlein, N., Vemaganti, K., and Anand, S. Bayesian Optimization of Energy-Absorbing Lattice Structures for Additive Manufacturing. pp. 12, 2020.

Johnson, L., Mahmoudi, M., Zhang, B., Seede, R., Huang, X., Maier, J. T., Maier, H. J., Karaman, I., Elwany, A., and Arróyave, R. Assessing printability maps in additive manufacturing of metal alloys. *Acta Materialia*, 176:199–210, September 2019. ISSN 1359-6454. doi: 10.1016/j.actamat.2019.07.005.

Kamath, C. and Fan, Y. J. Regression with small data sets: A case study using code surrogates in additive manufacturing. *Knowledge and Information Systems*, 57(2): 475–493, November 2018. ISSN 0219-1377, 0219-3116. doi: 10.1007/s10115-018-1174-1.

Lowther, M., Louth, S., Davey, A., Hussain, A., Ginestra, P., Carter, L., Eisenstein, N., Grover, L., and Cox, S. Clinical, industrial, and research perspectives on powder bed fusion additively manufactured metal implants. *Additive Manufacturing*, 28:565–584, August 2019. ISSN 22148604. doi: 10.1016/j.addma.2019.05.033.

Mindt, H. W., Megahed, M., Lavery, N. P., Holmes, M. A., and Brown, S. G. R. Powder Bed Layer Characteristics: The Overseen First-Order Process Input. *Metallurgical and Materials Transactions A*, 47(8):3811–3822, August 2016. ISSN 1543-1940. doi: 10.1007/s11661-016-3470-2.

Phua, A., Doblin, C., Owen, P., Davies, C. H. J., and Delaney, G. W. The effect of recoater geometry and speed on granular convection and size segregation in powder bed fusion. *Powder Technology*, August 2021. ISSN 0032-5910. doi: 10.1016/j.powtec.2021.08.058.

Phua, A., Cook, P. S., Davies, C. H. J., and Delaney, G. W. Powder Spreading over Realistic Laser Melted Surfaces in Metal Additive Manufacturing. *Additive Manufacturing Letters*, pp. 100039, February 2022a. ISSN 2772-3690. doi: 10.1016/j.addlet.2022.100039.

Phua, A., Davies, C. H. J., and Delaney, G. W. A digital twin hierarchy for metal additive manufacturing. *Computers in Industry*, 140:103667, September 2022b. ISSN 0166-3615. doi: 10.1016/j.compind.2022.103667.

Piascik, B., Vickers, J., Lowry, D., Scotti, S., Stewart, J., and Calomino, A. DRAFT Materials, structures, mechanical systems, and manufacturing roadmap. *NASA TA*, pp. 12–2, November 2010.

Rasmussen, C. E. and Williams, C. K. I. *Gaussian Processes for Machine Learning*. Adaptive Computation and Machine Learning. MIT Press, Cambridge, Mass, 2006. ISBN 978-0-262-18253-9.

Sames, W. J., List, F. A., Pannala, S., Dehoff, R. R., and Babu, S. S. The metallurgy and processing science of metal additive manufacturing. *International Materials Reviews*, 61(5):315–360, July 2016. ISSN 0950-6608, 1743-2804. doi: 10.1080/09506608.2015.1116649.

Samuel, M. P., Mishra, A. K., and Mishra, R. K. Additive Manufacturing of Ti-6Al-4V Aero Engine Parts: Qualification for Reliability. *Journal of Failure Analysis and Prevention*, 18(1):136–144, February 2018. ISSN 1547-7029, 1864-1245. doi: 10.1007/s11668-018-0393-9.

Scime, L. and Beuth, J. Using machine learning to identify in-situ melt pool signatures indicative of flaw formation in a laser powder bed fusion additive manufacturing process. *Additive Manufacturing*, 25:151–165, January 2019. ISSN 22148604. doi: 10.1016/j.addma.2018.11.010.

Shafto, M., Conroy, M., Doyle, R., Glaessgen, E., Kemp, C., LeMoigne, J., and Wang, L. DRAFT Modeling, simulation, information technology & processing roadmap. *National Aeronautics and Space Administration*, November 2010.

Tapia, G., Elwany, A., and Sang, H. Prediction of porosity in metal-based additive manufacturing using spatial Gaussian process models. *Additive Manufacturing*, 12:282–290, October 2016. ISSN 22148604. doi: 10.1016/j.addma.2016.05.009.

Tapia, G., King, W., Johnson, L., Arroyave, R., Karaman, I., and Elwany, A. Uncertainty Propagation Analysis of Computational Models in Laser Powder Bed Fusion Additive Manufacturing Using Polynomial Chaos Expansions. *Journal of Manufacturing Science and Engineering*, 140 (12):121006, December 2018. ISSN 1087-1357, 1528-8935. doi: 10.1115/1.4041179.

Tuegel, E. J., Ingraffea, A. R., Eason, T. G., and Spottswood, S. M. Reengineering Aircraft Structural Life Prediction Using a Digital Twin. *International Journal of Aerospace Engineering*, 2011:1–14, 2011. ISSN 1687-5966, 1687-5974. doi: 10.1155/2011/154798.

Wycisk, E., Solbach, A., Siddique, S., Herzog, D., Walther, F., and Emmelmann, C. Effects of Defects in Laser Additive Manufactured Ti-6Al-4V on Fatigue Properties.

Physics Procedia, 56:371–378, January 2014. ISSN 1875-3892. doi: 10.1016/j.phpro.2014.08.120.