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A Digital Twin Approach for the Prediction of the Geometry of Single Tracks Produced by Laser Metal Deposition

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Abstract

Flexible manufacturing processes such as laser metal deposition exhibit high potential for a production solely defined by software to cope with the current challenges of production systems. The determination of suitable machine parameters for the production of novel materials and geometries however requires extensive experimental effort. Existing simulative approaches do not offer sufficient accuracy to predict the relevant machine parameters in a satisfactory way. This paper presents a new concept, in which we apply a digital twin to provide a step towards a fully software-defined and predictable laser metal deposition process. The presented concept includes relevant data of the machines as well as data-driven machine learning models and physics-based simulation models. This enables a more reliable prediction of geometries of single tracks which was validated on a laser metal deposition machine.

Keywords: Laser metal deposition, Software defined manufacturing, Digital Twin, Asset Administration Shell

1. Introduction

Manufacturing companies face increasingly shorter product life cycles and the need for individualized products [1, 2]. Successful handling of these challenges requires flexible and reconfigurable manufacturing systems [3, 4]. This flexibility is expected to be manageable, if manufacturing systems are both universal and can be fully controlled by software, enabling what is commonly referred to as software-defined manufacturing [5].

Laser as a manufacturing tool offers high potential regarding flexibility, as it covers processes from all the six main groups of manufacturing processes defined in the DIN 8580 [6]. The laser metal deposition (LMD) process belongs to the group “primary forming”. It deposits several tracks of a given material one next to the other to form the desired three-dimensional part layer by layer. The geometry of a single track, which is characterized by its height and width, is influenced by the parameters of the LMD process. In the present paper, we focus on the freely selectable machine parameters laser power, supply rate of the powder, feeding speed, and diameter of the laser beam on the surface. To directly derive the machine code from a computer-aided design (CAD) file, a functional relationship between the machine parameters and the geometry

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of the produced tracks must be known. Deriving these functional relationships for a given LMD machine and a desired part is however a non-trivial task requiring a significant amount of skill and mostly manual effort.

To illustrate this, we consider different phases of the lifecycle of a machine and the respective experimental work. Initial estimations of the machine parameters are carried out by the manufacturer during production and commissioning of the machine. When the machine is handed over to the customer, most of the individual operator knowledge cannot be transferred to the new operator. Both the results and the efficiency therefore often vary strongly between manufacturer and customer, as well as between different customers and even between different operators at the same customer. The identification of functional relationships between machine parameters and geometry of a single LMD track is expected to overcome these drawbacks. Nevertheless, the complex interaction phenomena within the LMD processes limit the availability of analytical descriptions of the relationships between the machine parameters and the resulting track geometry [7].

Different analytical models were proposed by Cheikh et al. [8] and Ahsan et al. [9], while Zhang et al. [10] and Huang et al. [11] discuss implementations of numerical models. However, none of them is sufficiently accurate to predict the machine parameters without additional experimental validation. For instance, Cheikh et al. [8] assume unknown quantities, such as powder efficacy and absorption coefficient, while Ahsan et al. [9] do not consider thermophysical effects. A further approach uses data-driven models to predict the machine parameters [12]. In order to achieve applicability for a wide range of parameters and applications, sole focus on one machine is not sufficient. It is rather necessary to implement a more general concept for cross-machine collection and handling of data. Therefore, we opt for a digital twin (DT) of the process. While many different definitions of DTs are found [2, 4, 13], herein we refer to it as a virtual representation of the static and dynamic behavior of a real object, often referred to as an asset [2]. The DT contains all models and data of the represented object. It enables the virtual simulation of the physical behavior and it is continuously synchronized with the asset [2]. Consistency across the life cycle phases of the asset and thus across departmental and company boundaries is a fundamental property of DTs. Standardization and standardized interfaces are elementary for this purpose. One possible realization of the DT with a standardized framework is the asset administration shell (AAS) [13].

The application of DTs in laser material processing has already been addressed in some related work, e.g. on using DTs for defect-free production of components as reported by Gaikwad et al. [14], Stojanovic and Milenovic [15], and Papacharalampopoulos [16]. Knapp et al. [17] used a DT to predict the spatial and temporal distribution of the temperature and the resulting geometry of the LMD track. Prieto et al. [18] and Ertveldt et al. [19] present a framework for the collection, storage, preparation, and visualization of process data in the LMD process using DTs. The previously mentioned papers either do not predict the geometry of the produced tracks or solely base their prediction on numerical simulation. As of yet, there is no fully accessible concept for DTs in order to assist the estimation of parameters for LMD processes. We hence propose a novel concept of a DT to predict the geometry of the LMD tracks by providing data-driven and simulation models in a standardized and semantic way.

2. Concept

With the proposed concept, the machine manufacturer can additionally access operational data and predictions from the machine and the models via the DT to improve and test the models with a larger amount of more representative data. Figure 1 depicts our macroscopic concept which comprises several entities.

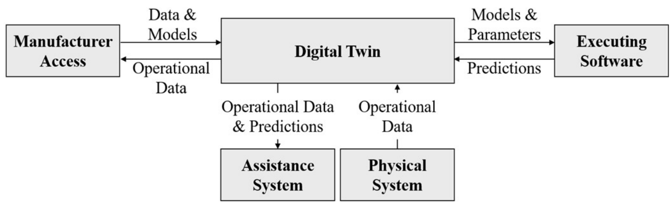

Figure 1: General concept

As the core of the concept, the DT contains several models, data, and interfaces to communicate with other entities and provides information to all parties involved in the process. A connection between the DT and the physical system - i.e. the LMD machine - allows for the collection of operational data and for storing it in the DT. The DT obtains various models and data about the physical system from the machine manufacturer through the manufacturer's access interface. The data contains general and technical information such as ranges of the machine parameters. The entity of the executing software runs the models provided by the DT and returns the predictions back to the DT. The assistance system, which is used by the machine operator, finally provides predictions of the geometry of the produced LMD tracks to help adapting the machine parameters.

Figure 2 shows the specific application of this concept including the processing workflow of LMD used for the additive manufacturing process. The LMD process starts with a CAD model, which includes local reinforcements that shall be printed together with the manufactured part. The computer aided design / computer aided manufacturing (CAD/CAM) program uses the CAD model to generate a code that is readable by the machine as a numerical control (NC) code. The geometry of the tracks is a requirement originating e.g. from the geometry of the part or requirements for the quality of the surface. The operator must provide the corresponding machine parameters to achieve the desired geometry and quality, where the assistance of the DT is needed. The physical system communicates with the DT through a physical system interface using e.g. an open platform communications – unified architecture (OPC-UA). Alternatively, one can use static values from the NC Code to determine the machine parameters used for the manufacturing process. The dimensions of the produced part are finally measured either manually or by automated measuring devices.

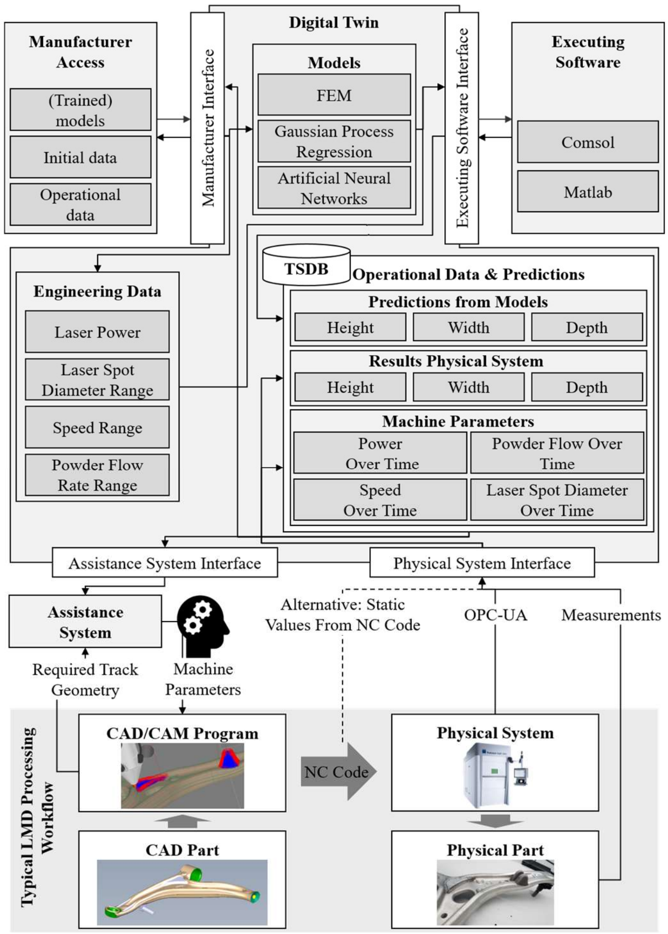

Figure 2: Concept of a digital twin for laser metal deposition

The data entered through the interface of the physical system are stored in the entity for operational data and predictions using time-series databases (TSDB). The results obtained by the physical systems, i.e. the measured geometry of the produced part, are also stored in this component. The prediction of the model using the parameters from the physical system is captured as well. These operational data and predictions are provided to the manufacturer through the manufacturer's interface as well as to the assistance system through the assistance system's interface. We use executing software such as COMSOL Multiphysics and MathWorks MATLAB to generate the predictions. The models are provided by the interface of the executing software are stored in the models component. Besides the models, we also provide the parameter ranges of the physical system, which is stored in the engineering data component, to the executing software. This engineering data is provided by the manufacturer through the manufacturer's access interface. The assistance system is provided with operational data and predictions through its interface to enable a quantitative or qualitative estimation of the track geometry depending on the parameters. The machine user can enter the machine parameters to the CAD/CAM program when the predicted geometry of the tracks suits the requirements. Other combinations of machine parameters must otherwise be explored to achieve the desired track geometry. These data are also provided to the manufacturer through the manufacturer's interface. The machine manufacturer can train and improve the provided data-driven and simulation models incrementally over time with this continuous collection of data from the physical system and the models. This leads to a more accurate prediction of the geometry of the single LMD-produced tracks.

3. Models and experimental data

An essential part of the proposed concept is to add simulation models besides the data-driven models to predict the geometry of the produced tracks.

3.1. Simulation models

A finite-element method (FEM) simulation model was implemented with the commercial software COMSOL Multiphysics. The model solves the transient heat-conduction equation to compute the heat transport by thermal conduction, convection, and radiation [20]. The latent heat was taken into consideration to account for the phase changes of the material [21]. Only a single additively produced bead was considered in the simulation in order to reduce computational time. The initial geometry was set to have a dimension of 10×3×1.5 mm, where the plane (0, y, z) was set to be symmetrical, so that only half of the geometry needs to be considered. The simulation time can thus be reduced and the variation of the temperature at the center of the geometry can be displayed. The ambient temperature and the initial temperature of the workpiece were set to 293 K. Thermal radiation and convection are applied at the top and bottom of the geometry. To model the increase of the volume caused by the supplied powder, a vertically moving mesh with the velocity v_{Z0} along the (0, z) direction was implemented on the upper side of the substrate. The velocity of the mesh mainly depends on the rate of the powder supply and can be described as proposed by Peyre et al. [22]. The heat source was implemented assuming a Gaussian laser beam at normal incidence and the related parameters: absorption coefficient A, laser power P_0 and radius ω_0 of the beam waist, which is located on the upper surface of the workpiece.

The exact value of A is afflicted with some uncertainty as it is affected by the exact condition of the irradiated material and was therefore used as a fitting parameter for calibration of the model with experimental data. The maximum mesh size was confined to 0.3 mm for the whole structure in order to improve the accuracy of the simulation and to obtain a sufficiently accurate calculation of the deformation. Automatic remeshing was implemented which occurs when the mesh quality, which is determined by measuring the skewness of the mesh as default in COMSOL, is below 0.1. The aluminum alloy AlSi10Mg was considered for the simulation with parameters taken from Chen et al. [23]. Figure 3 presents an example of the computed distribution of the temperature. The input parameters are the supply rate Q of the powder, the radius r_p of the powder stream, the feeding speed v, the laser beam parameters including the laser power P, and the diameter of the laser beam d. The distribution of the temperature on the workpiece is iteratively computed at each time step. The height of the layer is extracted by measuring the difference between the height of the deformed geometry and the original height of the geometry. The width and depth of the produced tracks are calculated without moving mesh only by solving the transient heat-conduction equation in a separated model solver. The simulated distribution of the temperature in the cross-section of the workpiece and the temperature at which the transition from liquid to solid occurs are considered.

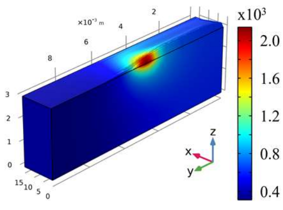

Figure 3: Exemplary temperature distribution calculated via FEM simulations

3.2. Data-driven models

Finding a functional relationship between the machine parameters and the geometry of the resulting tracks based on experimental data is a typical regression task, which can be implemented using various machine-learning approaches. In the following, we discuss the suitability of linear regression, tree regression, Gaussian process regression, and artificial neural networks for the given use case. The regression model needs to be able to handle the machine parameters as degrees of freedom and take into account the non-linear influence of the parameters on the process as well as their interrelated interactions. The experimentally determined values of the track geometry must be represented as accurately as possible, but at the same time, the regression model must be general enough to avoid overfitting.

In contrast to linear regression, tree regression is suitable for larger data sets and complex non-linear relationships. One major drawback of tree regression compared to linear regression is that it can neither discover trends nor extrapolate beyond the existing data [24]. Gaussian process regression is based on probabilistic functions and generally works well in the case of small datasets. It aims at maximizing the likelihood function and provides measurements of the uncertainty for prediction [25]. Artificial neural networks can be used for regression tasks [26]. As both artificial neural networks and Gaussian process regression are suitable for non-linear relationships between the various parameters, these algorithms are generally apt for our use case.

3.3. Experimental data

Experimental data was generated to train the data-driven models and to evaluate which of the previously mentioned models best represents our experimental results. The experiments were performed on the LMD machine TruLaserCell3000 with a 4 kW disc laser from TRUMPF GmbH + Co. KG using powder of AlSi10Mg with a distribution of the particle diameters ranging between 45 and 107 µm. The powder was conveyed to the process zone by means of a vibratory feeder, a helium gas flow, and a MultiJet-nozzle from TRUMPF. Single tracks with different machine parameters were welded on a 10 mm thick plate of AlMg3. Cross sections of the welding track, as exemplarily shown in Figure 4, were examined by means of an optical microscope.

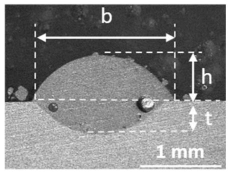

Figure 4: Cross-section of a single welding track; b is the width, h the height and t the depth of the track.

The laser power, the supply rate of the powder, the diameter of the laser beam on the surface, and the feed rate have a significant influence on the geometry of the resulting track. Therefore, these parameters were varied within broad ranges and variable step sizes: Laser power between 1 and 3.5 kW in 13 different steps, supply rate of the powder between 2.1 and 21 g/min in 11 steps, beam diameter between 1 and 2 mm in 4 steps, and feeding speed between 0.75 and 10 m/min in 8 steps. The experiments were repeated at least three times for each combination of the parameters, summing up to a total of 282 single tracks. A fraction of 80% of the gained data was randomly selected and used to train the models. Here, we applied k-fold cross-validation with five folds to tune the performance of the models. The remaining 20% of the data was used to test the performance of the data-driven models.

4. Results and discussion

For the implementation of the concept, the AASX-package explorer was used as a demo implementation of the AAS [4]. The AASX-package explorer is an open-source editor to create AAS provided by a publicly funded industrial consortium. The AAS ensures interoperability between machines and operational boundaries. This allowed obtaining the results presented and discussed in the following.

4.1. Validation of physical simulation models

Several simulations with different input parameters were executed to validate the physics-based simulation model. Three different laser powers, three different diameters of the beam and three different supply rates of the powder were considered. The absorption coefficient A was used as a fit parameter to adjust the model to the first set of experimental data, which resulted in A = 0.15 and was kept constant in the simulation. Table 1 compares the data-driven (Dat.) – using Gaussian process regression – and the simulated results (Sim.) with the experimentally measured values (Exp.) for some combinations of the machine parameters. As seen from Table 1, the height of the track, which is predicted by the simulation with the moving mesh, agrees well with the experimental measurements within a difference of up to 6%. The depth and width of the track were calculated without a moving mesh, as this delivered more accurate results. Thereby, the simulation results of the depth and the width still deviate from the experimental data within a difference of up to 14%. We explain this deviation as follows: Firstly, the material assumed in the simulation was the alloy AlSi10Mg whereas the experiments were carried out with the powder material AlSi10Mg on an AlMg3 substrate with a smaller thermal conductivity. Secondly, the fluid flow of the melt, which influences the shape of the formed bead [22], was not considered to save computational time. Thirdly, the absorption coefficient A was kept constant for all sets of parameters, even though the energy coupling into the material is expected to vary for different laser beam diameters.

Table 1: Validation of simulation and data-driven models with experimental data (white background). Input data marked with grey background

Laser power P (kW)		2.00	2.70	2.70	2.70	2.00
Laser beam diameter d (mm)		2.00	2.00	1.00	1.50	2.00
Powder supply rate Q (g/min)		3.10	3.10	3.10	2.80	3.10
Feeding speed v (m/min)		2.00	2.00	2.00	2.00	1.50
Track depth (mm)	Sim.	0.50	0.73	0.47	0.74	0.68
	Exp.	0.58	0.75	0.49	0.66	0.69
	Dat.	0.59	0.75	0.49	0.65	0.68
Track width (mm)	Sim.	1.89	2.61	2.17	2.35	2.52
	Exp.	2.10	2.68	2.26	2.35	2.48
	Dat.	2.15	2.66	2.24	2.35	2.42
Track height (mm)	Sim.	0.38	0.38	0.39	0.35	0.48
	Exp.	0.40	0.36	0.41	0.34	0.47
	Dat.	0.40	0.36	0.42	0.34	0.47

Despite the quantitative deviations between simulation and experimental data, the simulation displays the same trend as the experimental data for most of the investigated parameter changes: The spatial dimensions of the tracks increase with increasing laser power, the height of the track increases when the supply rate of the powder is increased, the width is decreased with decreasing beam diameter, and an increase of the feeding speed leads to a reduced height, width and depth of the track. Yet, the simulation gives no information about the influence of powder's supply rate on width and depth, as the moving mesh was not considered for the determination of these quantities.

4.2. Validation of data-driven models

The experimental data mentioned in Section 3.3 was compared to the results of the regression models mentioned in Section 3.2. The corresponding coefficients of determination with regard to the geometry of the tracks are summarized in Table 2. The width and the depth of the tracks are predicted comparably well by all models, but linear regression fails to predict the height of the tracks. This can be explained by the non-linear influence of the process parameters on the height of the tracks. Tree regression yields acceptable results for all geometrical dimensions, but height and depth are predicted less accurately than by means of Gaussian process regression and artificial neural networks. The latter two approaches yield the most accurate predictions and are thus both suitable for our use case. This can be explained by their ability to represent non-linear relationships and the better generalization of the data as compared to the other models. The validation of our proposed concept is exemplarily shown using Gaussian process regression in the following.

Table 2: Coefficient of determination R^2 for different regression models

Data-driven models	Track width b	Track height h	Track depth t
Linear Regression	R^2=0.85	R^2=0.58	R^2=0.90
Tree Regression	R^2=0.90	R^2=0.89	R^2=0.87
Gaussian Process Regression	R^2=0.90	R^2=0.95	R^2=0.95
Artificial Neural Networks	R^2=0.90	R^2=0.95	R^2=0.94

Figure 5 displays the experimentally determined width and height of the tracks and compares them to the values predicted by Gaussian process regression. Only the test data that has not been used for the training of the model is considered. Since the behavior of the depth of the track resembles that of the track's height it is not shown separately. The deviation between the measured and the predicted width of the track was smaller than 0.4 mm, respectively 22%. The deviation between the measured and the predicted height was less than 0.1 mm, respectively 23%, the one of the depth was smaller than 0.09 mm, respectively 14%. The process is robust enough to handle these deviations when parts are manufactured with a layer height in the order of 1 mm.

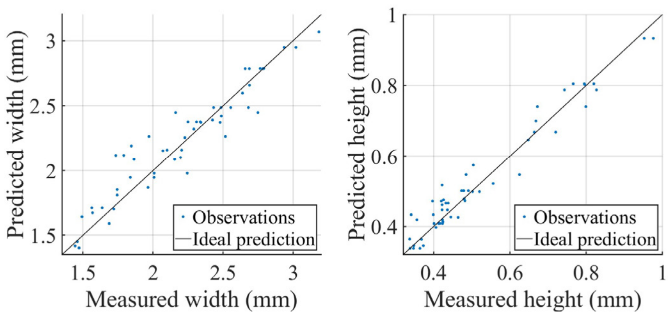

Figure 5: Comparison of predicted and measured values for track width (left) and track height (right) for Gaussian process regression

4.3. Discussion

As seen in Table 1, the predictions of the data-driven model and the simulation are generally in good agreement with the experimental data. It can however be clearly observed that the used data-driven models predict the track geometry more accurately than the physical simulation. Besides this, the simulation model has further drawbacks: Firstly, the absorption coefficient needs to be adjusted to fit experimental data. Secondly, the calculation time usually exceeds ten minutes compared to a prediction time in the range of seconds for data-driven models. Thirdly, the influence of the supply rate of the powder on width and depth of the track cannot be displayed.

This is because a moving mesh, which is needed to consider the effect of powder supply, was not used. Within the parameter ranges covered by training data, we therefore propose to predict the geometry of the track by means of data-driven models. The validation with 56 test data samples showed an accuracy within the same order of magnitude as the experimental uncertainty does. This accuracy allows planning of the tool path without preliminary experimental investigations, which is a significant contribution to a software-defined process.

However, data-driven models do not generalize well for parameter ranges that are not covered by training data. To show this, we applied our data-driven models with additional experimental data using a different range of machine parameters. Here, the data-driven models showed deviations of more than 50%. Physical simulation models can be generally applied and complement the data-driven models through qualitative predictions in these parameter ranges.

5. Conclusion and outlook

The use of digital twins in the field of laser metal deposition enables machine users to predict the geometry of single tracks using both data-driven and physical simulation models. By validating the data-driven models with experimental data, we proved that artificial neural networks and Gaussian process regression models are able to predict the geometry of the tracks accurately within the parameter ranges covered by training data. Moreover, our validation of the physical simulation models showed a qualitative agreement with the experimental results for most of the used machine parameters. These models, therefore, complement the data-driven models for parameter ranges that are not covered by training data. Our work shows the first combination of data-driven and physical simulation models in a digital twin for laser metal deposition. This offers a more accurate prediction of the track's geometry. In combination with data handling in the digital twin, it represents a promising step towards software-defined manufacturing.

Future studies are expected to extend data-driven models by additional parameters to achieve more versatility. In order to reduce the effort for data collection, automated acquisition of the height and width of the track is essential.

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