Optimization of process parameters for powder bed fusion additive manufacturing by combination of machine learning and finite element method: A conceptual framework

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Abstract

In addition to prototyping, Powder Bed Fusion (PBF) AM processes have lately been more widely used to manufacture end-use parts. These changes lead to necessity of higher requirements to quality of a final product. Optimization of process parameters is one of the ways to achieve desired quality of a part. Finite Element Method (FEM) and machine learning techniques are applied to evaluate and optimize AM process parameters. While FEM requires specific information, Machine Learning is based on big amounts of data. This paper provides a conceptual framework on combination of mathematical modelling and Machine Learning to avoid these issues.

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1. Introduction

Additive Manufacturing (AM) is “process of joining materials to make parts from 3D model data, usually layer upon layer, as opposed to subtractive manufacturing and formative” [1]. Development of new processes and materials provides a wider variety of areas for applications of AM. Nowadays, additive manufacturing is used not just in aerospace, medical and automotive industries but also in fashion, food industry, jewelry production and architecture, etc. [2]. With more use, more needs and requirements are set to products fabricated by additive manufacturing. One of the most difficult issues that should be addressed is how to improve and control quality of as-built part and define what significantly influence the quality level of a part.

Every additive manufacturing process has its own process parameters that in combination with material properties and environmental conditions influence quality of fabricated parts. Experimentally through the observation, it is very difficult to define those parameters and their combinations, which have the most impact on engineering (mechanical, physical and material) properties of the product. In addition, by the reason that practical experiments are expensive (especially for metal powder) [2], detecting parameters that influence quality of as-built part becomes more challenging task.

However, several studies can be found in the literature on application of Design of Experiments (DoE) methods (e.g. Taguchi, half-factorial design, central composite design, etc.) and analysis of variance (ANOVA) to define which parameters and their combination influence which type of properties of the as-built part [3-5].

Since statistical methods require big amount of data for more accurate results, just a few attempts were made comparing with general scientific attention to additive manufacturing. In addition to aforementioned studies focused on Taguchi, ANOVA and DoE methods, Garg, et al. [6] analyzed existing literature on application of empirical modelling for three AM processes (Stereolithography (SA), Selective Laser Sintering (SLS), and Fused Deposition Modeling (FDM)).

On the one hand, finite element modeling (FEM) is in most cases used for numerical solutions of mathematical models and parameters’ optimization, but this process requires deep knowledge on physical properties of material and in-depth understanding of AM process [7]. On the other hand, machine learning techniques can help to predict process parameters, thus avoiding the abovementioned...
requirements for FEM. Although these techniques normally require big amounts of data for better generalization and accuracy.

Combination of FEM and machine learning can provide possibility to simulate process (FEM), predict or optimize process parameters to achieve desired mechanical properties (Machine Learning), and then test predicted process parameters by testing them on developed models for process simulation (FEM).

Therefore, conceptual framework on combination of statistical analysis, mathematical modeling and machine learning techniques is proposed in this article.

2. Additive Manufacturing

2.1. Powder Bed Fusion Additive Manufacturing

According to ISO/ASTM52900-15 [1], powder bed fusion is “additive manufacturing process in which thermal energy selectively fuses regions of a powder bed”. This type of AM processes is widely used to manufacture parts and therefore, more research activities are focused on the improvements of the product properties (physical, material and mechanical properties). The schematic representation of powder bed fusion AM process is showed on Figure 1.

Additive manufacturing process always starts with machine preheating (up to 4 hours). Then process of powder solidification is performed by focusing laser on powder bed to fabricate one layer of designed part (Figure 1). Then powder bed moves down with a step of one layer thickness. The sequence of events should be repeated as many times as needed to build a part. After build is finished, machine should cool down before anyone can open the build chamber to take build cake out from it.

Metallic, ceramic, composite and polymer are types of material that can be fabricated by powder bed fusion additive manufacturing process. In addition, for metallic material, there are also 2 types of fusion source, which are electron beam and laser beam.

By the reason that during last decade more attention is paid to additive manufacturing and its development, there exist enormous amount of published literature about AM and powder bed fusion processes group. Therefore, this article is focused solely on polymer powder bed fusion (PPBF) process. However, other processes from this group should be investigated in the future work.

2.2. Application of statistical analysis to define significance of PPBF process parameters

Although there has been relatively little research on what AM process parameters are significant regarding final product quality, several studies reported results of statistical analysis for some AM process parameters. These attempts are based on application of such methods as Taguchi, ANOVA and regression modelling [6, 8, 9].

Singh and Prakash [10] planned experiment by application of two level factorial design of experiment (DOE) and evaluated which AM process parameters have significant impact on part density. Their analysis showed that among such parameters as laser power, scan spacing and scan velocity, the most significant is laser power. Based on ANOVA analysis, regression model was proposed including all significant factors and combinations of all three process parameters. Predicted density is in a good agreement with earlier published results [10].

Mousa [11] investigated influence of five process parameters on shrinkage phenomenon for glass bead-filled polyamide 12 samples fabricated by selective laser sintering. Application of DOE, Taguchi, S/N analysis and ANOVA methods led to the next results: powder base thickness has the most significant impact on shrinkage effect among such parameters as part bed temperature, laser power, powder base thickness, layer cooling time and filler ratio [11]. However, relationship between considered process parameters was not taken into account.

In addition, statistical analysis could be used for optimization and model development. Singh, et al. [12] presented study that is a good example of such application of statistical analysis. They optimized values of laser power, layer thickness, scan speed, and hatch spacing to achieve the best compressive strength without compromising porosity of open porous scaffold, which are fabricated from polyamide 12 by selective laser sintering process [12]. By application of ANOVA method, the authors were able to find regression model on the one hand, and evaluate significance of each parameter and their combination on the other hand. Laser power, layer thickness, hatch spacing and interaction between hatch spacing and laser power contributes the most to the value of compressive strength of scaffolds [12]. Based on the resulting regression model from ANOVA analysis, Singh, et al. [12] used trust region algorithm for parameters optimization. They validated results by fabricating and testing human skull, and comparing obtained results with the simulated one.

In addition, it is worth to mention that results from statistical analysis are also used to develop new mathematical description of powder bed fusion process.
3. Application of mathematical modeling for analysis of PBF AM processes

To be able to control quality of products produced by PPBF, there is a need in understanding of process and material behavior, and their interconnections. Therefore, mathematical modelling plays important role in finding solutions for this goal. However, all researchers emphasize the complexity of this task and the following challenges were mentioned in different articles [13-19]:

- Lack of understanding which parameters influence as-built parts
- Results differ from machine to machine, and from material to material, which makes it difficult to generalize proposed solutions
- Lack of information about physical properties for polymer powder used by PPBF (e.g., polyamide 12)
- Scientists need to have deep knowledge about both process and material to be able mathematically describe different phases in the process
- Too complex mathematical descriptions that require a lot of power, time and money to be solved

To meet these challenges, finite element modelling (FEM) and analysis (FEA) is used to find numerical solution for developed mathematical models. There are three different levels of model complexity: 1D, 2D or 3D modeling.

While one-dimension FE models were created by Nelson, et al. [20] to describe mathematically heat transfer of PBF process, Singh and Prakash [10] applied two-dimensional finite element analysis to predict average density of parts that can be fabricated by SLS AM process. They were also focused on simulation of heat transfer for one layer of a build. Two-dimensional model was based on such parameters as time, initial temperature of sintering, layer thickness, average powder density, laser beam diameter and width of raster line. According to authors [10], predicted values of average density of part is in a good agreement with previously published results.

Another example of simulation of polymer powder bed fusion process but in more complex way, namely 3D modeling, were presented by Bugeda, et al. [16]. The authors developed a model for 3D simulation of selective laser sintering process of polycarbonate in terms of temperature and density distributions. This model consists of thermal and sintering submodels, which used as input parameters laser beam intensity, radius and beam velocity, thermal properties (conductivity of solid material and air), rheological properties (initial solid fraction, activation energy and viscosity), and geometrical variables (positions of the heat source and powder bed dimensions) [16].

Chen, et al. [21] in their work simulated dynamics of bead formation, shape of melt pool and shrinkage consolidation using finite element modeling. Among all necessary parameters for numerical model solution, authors used two types of parameters related to the additive manufacturing. The first group of parameters are AM machine-related: layer thickness, temperature, laser power, beam radius, and reflection coefficient at bed powder surface. Another group of parameters is material-related: material local density and velocity, conductivity and dynamic viscosity.

Dong, et al. [17] simulated selective sintering process by development of 3D finite element model. The main goal was set to simulation of temperature and density distributions on powder bed, and analysis of effect of scanning speed, intensity of the laser, preheating temperature and spot size of laser beam on selective sintering process. However, polycarbonate powder was investigated due to lack of information about physical properties of other types of material [17]. Another attempt to simulate selective laser sintering process and better understand behavior of amorphous polycarbonate by using was done by Dong, et al. [13] through development of 3D transient finite element model.

Kumaresan, et al. [14] made the static structural analysis of four different scaffold models. Authors applied FEA to simulate stress concentration for cubical, shifted cubical, spherical and shifted spherical models based on such parameters as porosity ranges, pore size, pore interconnectivity, load bearing capacity and ease of cell penetration [14]. Shifted cubical model appeared to be the best model among others.

Ganci, et al. [15] developed 3D thermal model that allowed to predict temperature fields and extension of the sintered area in polymer powder bed for polypropylene. Josupeit, et al. [18] proposed simplified version of thermal finite element model for temperature and heat flow during cooling phase. Eshraghi and Das [19] proposed micromechanical FEA model of composite (polycopro lactone-hydroxyapatite, PCL:HA) scaffolds produced by SLS process. Their model was developed starting from 1D random sphere packing model through 2D micromechanical FEA model resulting in 3D macroscale model for different 3D model scaffold designs. The main purpose of this research was to find the best material ratio of PCL:HA with highest compressive strength. As authors reported that previous research on simulation of compressive testing of pure polycopro lactone (PCL) had disagreement with experimental results (from 67% to 100%), but their results showed just 26% of error and should be further improved.

As it can be summarized from the literature review presented in this chapter, mathematical modeling in combination with FEA is widely used to simulate sintering process, improve design of the product based on different requirements, and in some cases for optimization of value of layer thickness, laser power, scan speed, etc. Schematic representation of process/material parameters used to simulate sintering process and optimize values of process/material parameters are presented on Fig. 3.

However, modelling of the whole sintering process is a complex task, and requires information and data on physical properties and parameters, which influence is not fully described at this moment. Therefore, accuracy of proposed model should be further improved and the associated work should be more focused on the modelling of pre-heating and fabrication of parts including material phase changes.
4. Application of Machine Learning for prediction of PBF process parameters

The results of application of machine learning for additive manufacturing were reported for the first time in literature over 20 years ago [31], and nevertheless limited amount of published research studies is available nowadays. One can make a few assumptions to explain this situation:

- ML requires a big amount of data for accurate performance;
- expensive experiments (material costs) and therefore hard to gather enough data;
- not all articles were found due to earlier limit of standard for AM terminology, and regularly scientists use different synonymous for the same process;
- not all articles have in the title or key words “machine learning” or its methods but in text it is described to what extent ML methods are used for; etc.

Among all found articles focused on machine learning application, three dimensional bin-packing problem with nonconvex parts having holes and cavities to be fabricated by Stereolithography AM process were the first problem described using genetic algorithm for optimization of parts orientation [31]. According to Garg, et al. [6] review on application of machine learning or statistical methods for layer-based rapid prototyping, the most attention was paid to Fused Deposition Modelling (FDM) AM process until year 2014. Although one can argue that their review looks into limited amount of types of AM process, and a comprehensive review is required.

However, because this article is focused just on application of machine learning methods for polymer powder bed fusion process, review of other additive manufacturing processes is not included in this article and can be found elsewhere.

4.1. Machine Learning application for polymer powder bed fusion AM process

Many attempts are done to understand behavior of various materials suitable for PPBF AM process, and modeling was used as a main technique. AM processes are simulated and process parameters are optimized by developing different mathematical models and then solving them numerically (mainly FEM). However, many scientists reports that this is complicated task and results depends on the precision of finite element model [30].

Therefore, scientists started using and evaluating different machine learning techniques towards modelling and simulation of AM processes. Machine learning methods and their combinations, which are applied for simulation of PPBF AM process at this moment, are described in the literature [22-30]:

- Artificial neural network
  - Back propagation neural network
  - Radial basic function neural network based on fuzzy clustering and Pseudo-Inverse method
- Genetic Algorithm
  - Multi-gene genetic programming (MGGP)
  - Non-dominated genetic algorithm (NSGA-II)
  - Multi-objective particle swarm optimizer
- Ensemble-MGGP that consists of ANN, Bayesian classifier and Support Vector Machine algorithm
- Support Vector Regression (SVR)

Artificial Neural Network (NN), mainly back propagation NN, and Genetic Algorithm (GA) are the most used machine learning methods for process modelling, optimization and prediction of process parameters. For instance, Rong-Ji, et al. [27] made an attempt to determine the best process parameters to fabricate parts with higher level of accuracy. Authors focused on such parameters of SLS as the layer thickness, hatch spacing, scanning speed, scanning mode, laser power, interval time, and work surrounding temperature. To obtain optimum process parameters listed above, Rong-Ji, et al. [27] applied combination of genetic algorithm and back propagation (BP) NN algorithm. In this study results from BPNN was used as input parameters for fitness function in GA. Genetic algorithm was used as a method to determine optimal process parameters based on minimum shrinkage ratio [27]. Basic principle of BPNN were well described in [32], and Garg, et al. [6] present description of GA.

Literature review showed that almost all studies used from 16-50 samples as an input for both ANN and GA. Although, it is well-known that ML methods require a big amount of data, hence neural network will be more accurate and issues of overfitting the model can be avoided. Thus, one can argue that results based on 16 samples are valid, and therefore this issue should be taken into account in the future.

However, just one article is among all reviewed that developed algorithm based on over 100 samples. Munguia, et al. [29] applied neural network to estimate build time and relevant costs namely labor, machine costs and overheads. Their algorithm was developed on 130 samples, 90 of them were used for training, 25 for validation and 15 for testing.

The schematic representation of relationship between process parameters (input) and part’s properties defined by application of artificial neural network are presented on Fig. 3. Fig. 3 shows that shrinkage ratio and density parameters are dependent on the more than 10 and 6 process parameters, respectively. However, this is based on the scientists’ preferences and choice, and more process parameters should be inveiglated towards variations in mechanical and physical properties of a part. In addition, articles focused on genetic algorithm application is not presented on the Fig. 3. Just a few articles [22, 23, 33] are...
published on application of GA to optimize process parameters of polymer powder bed fusion system. Garg and Lam [23] made attempt to measure environmental aspect of 3-D printing by application of ANN, Genetic Programming and Support Vector Regression (SVR) methods. However, one can argue that mentioning that polymer powder used by SLS process reduces waste and saves fuel due to it is biodegradable is enough to make statements on environmental aspects of sustainability. Their results [23] showed that genetic programming performance is better than the other two, however how open porosity is connected to measurements of environmental aspects is unclear.

Garg, et al. [22] investigated prediction of open porosity for SLS fabricated parts from self-made powder as a mix of hydroxyapatite (HA) and polyamide (PA). In addition, they applied multi-gene genetic programming algorithm (MGGP) and ensemble-MGGP (EN-MGGP). More information about methods and process of powder preparation can be found in their article [22]. Results showed that layer thickness, laser power and laser scan speed has significant impact on open porosity, and EN-MGGP is better that classical MGGP algorithm.

Padhye and Deb [33] tested and evaluated different methods for multi-objective optimization and multi-criteria decision making. They borrowed already described by other scientist two multi-objective evolutionary algorithms that are non-dominated sorting genetic algorithm (NSGA-II) and multi-objective particle swarm optimizer (MOPSO), and tested them on 16 different 3D CAD models considering surface roughness and build time as main parameters that should be minimized [33]. Their results showed that there is some shapes that do not have one best solution, while for other shapes NSGA-II found better optimization solution. However, authors mentioned that this work hasn’t been experimentally verified, and should be done in the future.

All presented studies have a few aspects in common. First of all, application of machine learning methods is motivated by a few reasons: lack of understanding of parameters and especially their combinations that may influence on engineering properties of a part, and how it can be described through mathematical models including physical properties of polymers with high precision.

Second of all, the small data sets due to high costs of powder and expensive production of samples are another reason why proposed algorithms may have issues of generalization of results.

5. Proposed conceptual framework on combination of Machine Learning and mathematical modeling

Different techniques on analysis, modeling and simulation of polymer powder bed fusion process are presented above. However, all of these methods require practical experiments first to gather data that later is used for analysis, modelling or simulation. In case of statistical analysis, data is used to define either significance of process/material parameters related to product quality, or regression models that mathematically describes relationship between process parameters, their interconnection and quality of product or other desired output.

Finite element modeling/analysis is mainly used to simulate physical processes that are performed during fabrication of parts by PPBF process. This is caused by the need in deep understanding of additive manufacturing process behavior including material changes during process. However, this type of AM process analysis is very complex because many physical laws should be applied to describe changes in the process, and thus, amount of coefficients used in physical laws very often leads to limitations and simplifications of mathematical description due to lack of information, especially for newly developed materials.

Therefore, latest research is focused more on machine learning methods that can help to avoid this challenge. Machine learning allows optimizing process/material parameters by prediction of desired engineering properties of product, and the most important part of this type of optimization is that input variables are all available parameters that can be controlled and changed in AM process and material.

In all three cases, data from practical experiment is used either for one of the methods or for combination of two of all described methods (statistical analysis with FEM [18], statistical analysis with machine learning [34] or FEM and machine learning [35]). These combinations already showed that application of mixed methods allows improvements of quality of final product that are very important for production lines in the industry.

Inspired by Ma, et al. [36] work, generalized conceptual framework on combination of machine learning, statistical analysis and mathematical modelling with consideration of a particular additive manufacturing process and type of material is proposed in this paper as a possible solution of abovedescribed challenges and is shown on Fig. 4.

One of examples, how this combination is beneficial is demonstrated below. For instance, Design of Experiments can be applied for better understanding of which process and material parameters (their combination) have the most impact on mechanical properties. Then, results from this analysis can be used partly as an input for mathematical models to be solved by FEM and partly as an input in Machine Learning algorithm. The latter one can be coupled with the mathematical model developed for finite element analysis as a fitness function in ML techniques.
6. Conclusion

This paper presents review of three methods that are used to control and manage quality of parts produced by PPBF AM process. Review showed that statistical analysis as well as machine learning requires big amount of data to be more accurate. In contradiction, mathematical modeling requires deep knowledge on both process and material physics. Proposed conceptual framework provides an idea of how these challenges can be avoided. By the reason that all methods use the similar type of input, their combination is possible without any additional costs. Another benefit is a generalized perspective on all AM processes that was built upon PPBF process. In the future work, more attention will be paid to practical realization of a proposed framework.

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