Optimization of fused filament fabrication process parameters under uncertainty to maximize part geometry accuracy

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Abstract

This work presents a novel process design optimization framework for additive manufacturing (AM) by integrating physics-informed computational simulation models with experimental observations. The proposed framework is implemented to optimize the process parameters such as extrusion temperature, extrusion velocity, and layer thickness in the fused filament fabrication (FFF) AM process, in order to reduce the variability in the geometry of the manufactured part. A coupled thermo-mechanical model is first developed to simulate the FFF process. The temperature history obtained from the heat transfer analysis is then used as input for the mechanical deformation analysis to predict the dimensional inaccuracy of the additively manufactured part. The simulation model is then corrected based on experimental observations through Bayesian calibration of the model discrepancy to make it more accurately represent the actual manufacturing process. Based on the corrected prediction model, a robustness-based design optimization problem is formulated to optimize the process parameters, while accounting for multiple sources of uncertainty in the manufacturing process, process models, and measurements. Physical experiments are conducted to verify the effectiveness of the proposed optimization framework.

Keywords: Additive manufacturing, Material extrusion, Fused filament fabrication, Process design, Experimental validation

1. Introduction

Multiple sources of variability and uncertainty in each stage of the manufacturing process contribute towards the product variability and quality [1], thus restricting the application of AM. The effect of process parameters on product quality has been studied extensively. Armillotta et al. [2] studied the edge quality in FFF by building parts with varying inclination,
included angle and incidence angle. Alafaghani and Qattawi [3] investigated the effects of infill percentage, infill pattern, layer thickness, and extrusion temperature on dimensional accuracy using Taguchi design of experiment method. Variation of mechanical properties over a range of build orientation, layer thickness and feed rate was analyzed by Chacón et al. [4]. These studies use an experiment-based trial-and-error approach for the selection of process parameters, which consumes time and resources, wastes material and energy, and still does not explore all the possibilities. Thus, instead of physical experiments, simulations using a computational model would be more economical in exploring a wide range of process parameter settings and their effects on the AM product quality.

However, AM is a complicated process and the physics models may not adequately capture all the physical phenomena associated with the different stages of AM. Several physics models are available in the literature depending on the quantity of interest (QoI) related to product quality, and the process parameters that can be controlled. Ahn et al. [5] proposed a theoretical expression for surface roughness and studied the effect of process parameters such as surface angle, layer thickness, filament cross-section shape, and overlap interval on surface roughness. For the study of part distortion, finite element (FE) analysis has been used as a predictive model [6–8] and the predictions compared with experiments. Xia et al. [9] used finite-volume/front tracking method to solve the governing conservation equation for polymer flow and tracking the interface and studied the effect of temperature and spacing of the filaments on the shape of the final product. An adaptable three-dimensional transient model with a boundary-adjusting finite difference method for predicting the temperature field of the deposited layer was presented by Zhang et al. [10]. These studies focus specifically on the development of the physics model and its improvement by considering better constitutive models, meshing strategies, etc.

Refining the measurement techniques to collect good quality data has been the focus of other studies. Real-time monitoring of strain and temperature data from embedded fiber Bragg grating sensors and thermocouples was studied by Kousitza et al [11]. Infrared thermal cameras are used to record the temperature field [12]. Zhou and Hseih [13] developed a numerical method to apply infrared thermography to suit the complications caused by the material phase changes in FFF. For measuring the dimensional accuracy and surface roughness, calipers and 3D scanners have been used [14]. Denlinger et al. [15] studied the effect of dwell time on part distortion, measured using a laser displacement sensor.

In addition to the physical variability in the AM processes, the use of numerical models of
AM processes introduce additional uncertainty sources (both aleatory and epistemic) such as model parameter uncertainty due to lack of knowledge about the model parameters, numerical solution error due to truncation error, discretization error, etc., and model form error due to assumptions and simplifications in the modeling. Experimental observations also have uncertainty due to process variability and measurement errors. The effects of these uncertainty and variability sources on the QoI prediction can be investigated through systematic uncertainty quantification (UQ) techniques. However, multiple runs of the numerical model are needed in UQ analysis. Therefore, expensive numerical models are often replaced by cheaper surrogate models, which introduces an additional surrogate model error. The above uncertainties need to be systematically considered while optimizing the process parameters, requiring formal methods for optimization under uncertainty. Recently, some studies have explored deterministic approaches towards design for additive manufacturing (DfAM). Abid et al. [16] proposed a response surface model to evaluate the effects of manufacturing direction and deposition angle on the mechanical properties such as Young’s modulus, yield stress, and tensile strength. Asadollahi-Yazdi et al. [17] proposed a DfAM approach for the selection of process parameters using a multi-objective formulation to optimize the mechanical properties and product roughness. Liu et al. [18] addressed the problem of concurrent deposition path planning and structural topology optimization. These studies did not consider design under uncertainty. Wang et al. [19] presented a robustness-based design optimization approach for the process parameters in metallic AM focused on maximizing equiaxed grains in the microstructure; however, this work did not address model uncertainty or consider conflicting objectives.

In this paper, we propose a systematic methodology to optimize the AM process parameters while accounting for multiple uncertainty sources in manufacturing, physics modeling, and measurements. Specific contributions are made in the following individual steps: (1) A multi-physics simulation model is constructed for the FFF process to connect the process parameters to the QoIs, and the various sources of uncertainty in the simulation model are incorporated. The thermal model is first coupled with the mechanical model to simulate part deformation. (2) The uncertainties arising from different sources in the manufacturing process, physics modeling, and measurements are quantified and aggregated. A surrogate model is employed to reduce the computational effort in UQ, which is then corrected using experimental observations to make it more accurately represent the physics of the actual manufacturing process. (3) An optimization problem is then defined and solved to arrive at the optimal process parameters with the objective
of minimizing the geometric inaccuracy of the manufactured part.

The remainder of the paper is organized as follows. Section 2 discusses physics-based models of the FFF process used in this paper. The proposed methodology for process parameter design is outlined in Section 3. The process optimization methodology is illustrated through a numerical example in Section 4, and concluding remarks are provided in Section 5.

2. Physics models of the FFF process

This section describes the physics-based models used in this paper. A very brief survey of available modeling options was provided in Section 1. FFF is an extrusion-based AM technique generally used for plastics and polymers. In this work, the thermo-mechanical process of FFF is simulated using two models: (a) Thermal model for heat transfer analysis, and (b) Mechanical model for structural deformation analysis. The models are one-way coupled (or weakly coupled) [7], where the temperature history generated in the thermal model is imported as heat load into the mechanical model to estimate the deformation and hence predict the manufactured geometry (Fig. 1). Similar thermo-mechanical models have been used in previous studies [6, 8] and have shown good agreement with experiments. Note that the focus of this paper is to develop and demonstrate the methodology for process parameter optimization under uncertainty. The physics models used in this demonstration can be replaced by more sophisticated models if desired. However, that will greatly increase the computational effort in UQ and optimization. Also, a main component of the proposed framework is the calibration of model discrepancy (Section 3.2.2), i.e., estimating the error due to simplifications and assumptions in the physics model. For example, the thermo-mechanical model (Section 2) ignores the contribution of voids to the dimensional inaccuracy of the part. However, since we explicitly account for the model error by quantifying the model discrepancy and including it in the optimization, the thermo-mechanical model might be adequate for optimization purposes. After the optimization, more sophisticated models that include volume shrinkage, fluid dynamics and viscoelasticity can be used for accurate prediction and assessment of the optimum solution.

2.1. Thermal model for heat transfer analysis

The thermal model shown in Fig. 1 performs the heat transfer analysis of the AM process. The inputs to the model are the process parameters and the thermal properties, and the output is the spatio-temporal temperature field. The governing equation for the heat transfer analysis
is given by Eq. (1):

\[
\frac{\partial (\rho C_p T)}{\partial t} = \nabla \cdot (k_c \nabla T) + Q
\]

(1)

where \( T, t, \rho, C_p, k_c, Q \) are temperature, time, density, specific heat, thermal conductivity, and the internal heat generated. The extrusion process of FFF is modeled by element deactivation-activation. All the elements are initially deactivated. Addition of extruded material is simulated by activating the elements one-by-one. Multiple ways of extrusion are discussed later in Section 3.1.1. The initial temperature of the extruded material is set at the nozzle temperature. The build plate temperature is applied as a fixed boundary condition at the bottom surface of elements in contact with the build plate. The convection and radiation boundary conditions at the outer surfaces of the part are set as follows:

\[
q_c = h(T - T_{amb})
\]

(2)

\[
q_r = K_b \varepsilon_{em}(T^4 - T_{amb}^4)
\]

(3)

where \( q_c, q_r, h, T_{amb}, \varepsilon_{em}, \) and \( K_b \) are heat flux due to convection, heat flux due to radiation, the heat convection coefficient, the envelope temperature of the chamber, emissivity, and the Stefan-Boltzman constant respectively. The heat transfer analysis is performed in Abaqus [21], and the temperature field at the nodal locations for every time step is recorded. This temperature field is the input to the mechanical model.

2.2. Mechanical model for structural deformation analysis

Rapid heating and cooling during extrusion leads to residual stresses and deformation. The associated physical phenomena are heat transfer and stress equilibrium. The heat transfer is
handled by the thermal model described above. The mechanical model in Fig. 1 performs the structural deformation analysis. Process parameters, mechanical properties, and temperature field from the thermal model are the inputs to the mechanical model; and nodal deformation is the output. The total strain $\varepsilon_{\text{total}}$ is given by [22]

$$
\varepsilon_{\text{total}} = \varepsilon^e + \varepsilon^th + \varepsilon^pl
$$

where $\varepsilon^e$, $\varepsilon^th$, and $\varepsilon^pl$ are the elastic, thermal, and plastic strain components respectively. The governing equation for mechanical analysis [23] is given by

$$
\nabla \cdot \sigma + f = 0
$$

where $\sigma$ and $f$ are the stress tensor and internal forces. Considering elasto-plastic behavior typical for polymers and plastics, from Hooke’s law,

$$
\varepsilon^e = C^{-1}\sigma
$$

where $C$ is the material stiffness tensor. In this work, we are mainly concerned with the thermal loads. Thermal strain can be calculated from the thermal expansion constitutive equation:

$$
\varepsilon^th = \alpha_{th}\Delta T
$$

where $\alpha_{th}$ is the thermal expansion coefficient and $\Delta T$ is the change in temperature. The plastic strain is given by

$$
\varepsilon^pl = g(\sigma_Y)
$$

where $g$ is a function representing material behavior and $\sigma_Y$ is the yield stress. Elastic-perfectly plastic model is used in this work [8]. The above model is implemented in Abaqus. The nodal temperature history generated in the thermal model is imported as a predefined field into the mechanical model which calculates the deformation of the part.

2.3. Coupling of the models

The heat transfer and structural deformation analyses described in the previous subsections need to be coupled to numerically represent the FFF process. Typically, the numerical model
of FFF is represented by a weakly coupled analysis [6, 8]; the temperature field is computed first as the output of the thermal model, which is then applied to the mechanical model as thermal loading to calculate the residual stresses and deformations. This approach is cheaper as it requires only one run of each model during each time step, as opposed to multiple runs to convergence in each time step in a fully coupled analysis [24].

3. Proposed Methodology

This section presents the methodology to optimize the AM process parameters with a focus on FFF. The methodology presented in this section is general and applicable to any AM technique by using the corresponding numerical models and experiments. The proposed method consists of three main components: (a) Modeling of the AM process, (b) Uncertainty quantification, by integrating model prediction and experimental observations, and (c) Process design optimization under uncertainty. Multi-physics models described in Section 2 are linked to simulate the FFF process. Since the coupled physics model is expensive to simulate, a cost-benefit analysis is first carried out with regard to the approximation of the extrusion process, and then replaced with an inexpensive surrogate model to further reduce the computation cost. The model prediction is compared with experimental observations, and is corrected by adding a discrepancy term to the prediction. Then, an optimization problem to select the optimal process parameters is formulated and solved.

3.1. Modeling of the AM process

The physics-based models for FFF described in Section 2 are used in this work. However, the optimization of process parameters requires repeated evaluations of the physics-based simulation models by varying the process parameters, and these computational models are expensive to simulate. For example, Cattenone et al. [6] conducted an FE analysis of a planar spring (40 mm × 65 mm) on an Intel Core i7-6700 CPU 3.4 GHz machine, 16GB RAM employing parallel computing with 4 CPUs. The computational time for the thermal and mechanical analyses with 16400 finite elements were reported as 300 minutes and 900 minutes respectively. Realistic parts of larger size with complicated geometry will greatly increase the computational effort. Parallel computing can help in reducing the computation time. However, the speedup is leveled off by the overhead due to communications and data transfer between the CPUs as the number
of processors is increased. Therefore we implement two strategies for reducing the computation cost, namely material extrusion approximation and surrogate modeling, as described below.

3.1.1. Material extrusion approximation

The material extrusion and deposition process mentioned in Section 2 can be approximated in three ways depending on the size of the elements being activated, namely, (a) nozzle diameter, (b) raster lines, or (c) layers as shown in Fig. 2.

![Figure 2: Extrusion of FFF process approximated to (a) nozzle diameter, (b) raster lines, and (c) layers]

Though approximating and activating the elements of the size of nozzle diameter is considered to closely approximate the actual physical process, it can be expensive. Consider the simulation of a part 4.8 mm × 4.8 mm × 1.4 mm sliced into two layers of thickness 0.7 mm. This part is simulated by discretizing the extrusion process in the three ways mentioned above (Fig. 2). The output QoIs from both the models (temperature from the thermal model and part thickness from the mechanical model) at the last step of the simulation are plotted in Fig. 3 along a section perpendicular to the nozzle path (AA’ in Fig. 2c) at the top surface.

![Figure 3: Comparison of QoI from (a) the thermal model and (b) the mechanical model for different approximations of the extrusion process]
As shown in Fig. 3, the difference between the extrusion approximation as nozzle diameter and raster lines is not significant, whereas the layer approximation gives a significantly different result. However, using a desktop computer with Intel® Core™ i7-4790 CPU@3.60 GHz with 16GB RAM, it is shown in Table 1 that the difference in runtime between the nozzle diameter and raster line approximations is significant. Activating the elements as raster lines appears to give the best tradeoff between accuracy and computational effort. Note that as the size of the part increases, the runtime increases rapidly, hence multiple runs for the UQ analysis become infeasible; therefore, an activation strategy with a reduced computational effort is needed while not sacrificing too much accuracy. Further, this approximation will be captured by the model discrepancy term as mentioned Section 3.2.2.

<table>
<thead>
<tr>
<th></th>
<th>Thermal</th>
<th>Mechanical</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drops</td>
<td>210s</td>
<td>347s</td>
</tr>
<tr>
<td>Lines</td>
<td>37s</td>
<td>54s</td>
</tr>
<tr>
<td>Layers</td>
<td>19s</td>
<td>21s</td>
</tr>
</tbody>
</table>

3.1.2. Surrogate modeling

Even with material extrusion as raster lines, the computation cost is high for realistic parts. Therefore, the use of surrogate models to replace the physics-based simulation models to further reduce the computation cost becomes necessary. Different kinds of surrogate modeling techniques are available, such as polynomial chaos expansion, Gaussian process, radial basis functions, etc. In this paper, a Kriging surrogate model (i.e., Gaussian process model) is used.

A computationally expensive simulation model $G(d)$ with input $d$ is approximated to an inexpensive function $\hat{G}(d)$ by a Kriging model [25, 26] as

$$\hat{G}(d) = \alpha(d)^T \beta + \gamma(d)$$

where the trend part consists of the trend functions $\alpha(d)$ and trend coefficients $\beta$; and $\gamma(d)$ is a zero mean Gaussian process with covariance $Cov[\gamma(d_i), \gamma(d_j)] = \sigma_\gamma^2 K(d_i, d_j)$, for process variance $\sigma_\gamma^2$ and correlation function $K(\cdot, \cdot)$. The Kriging model is trained with $n_t$ observations.

Defining $G = [G(d_1), G(d_2), \ldots, G(d_{n_t})]^T$, $A = [\alpha(d_1), \alpha(d_2), \ldots, \alpha(d_{n_t})]^T$, and $K(d_i, d_j)$, $i, j = 1, 2, \ldots, n_t$ as elements of correlation matrix $K$, the trend coefficients are given as $\beta = (A^T K^{-1} A)^{-1} A^T K^{-1} G$. The mean and variance of the prediction at an untrained point $d_*$,
are given by
\[
\mu(d_*) = \beta^T (d_*) \beta + K\beta K^{-1} (G - A\beta)
\]  
(10)

\[
\sigma^2_\gamma = \frac{(G - A\alpha)^T K^{-1} (G - A\alpha)}{n_t}
\]  
(11)

The accuracy of the surrogate model depends on the number and locations of the training points. In this work, surrogate model error is quantified by evaluating the mean absolute percentage error (MAPE) using the leave-one-out (LOO) cross-validation (CV) technique. In LOOCV, \((n_t - 1)\) data points are used to train the surrogate model \(\hat{G}(d)\) in Eq. 9 and the remaining data point is used to test the surrogate model. The error metric defined as the MAPE value \(V_m\) is given by
\[
V_m = \frac{1}{n_t} \sum_{i=1}^{n_t} \left| \frac{G(d)^i - \hat{G}(d)^i}{G(d)^i} \right|
\]  
(12)

If the MAPE value is less than a user-defined tolerance, the surrogate model is deemed fit to be used for further analysis. Otherwise, more training points need to be added to improve the surrogate model accuracy. Adaptive training approaches such as efficient global reliability analysis (EGRA) [27], adaptive Kriging Monte Carlo simulation (AK-MCS) [28], prediction bias minimization [29], and global sensitivity analysis-enhanced surrogate (GSAS) [30] can be employed to adaptively locate training points that maximize the useful information from the training runs when the computational resources are limited.

3.2. Uncertainty quantification

This section discusses UQ in AM, by integrating model prediction and experimental observations.

3.2.1. Uncertainty sources

Uncertainty sources can be classified into two categories: (a) \textit{Epistemic uncertainty} due to lack of knowledge, and (b) \textit{Aleatory uncertainty} due to natural variability. \textit{Epistemic uncertainty} is subdivided into \textit{model uncertainty} and \textit{data uncertainty}. \textit{Model uncertainty} is caused by uncertainty regarding model parameters, model form error, and solution approximation error. \textit{Model parameters} such as material properties (conductivity, density, specific heat, etc.), plasticity model parameters, damage model parameters etc. are considered uncertain when the true value is unknown or cannot be determined with absolute certainty. \textit{Model form error}
is caused by the assumptions and simplifications made in developing the mathematical model (governing equations) of the physical system or process such as approximation of material extrusion and deposition as discrete elements in FFF, approximation of the shape of the grain as a square in laser powder bed fusion (L-PBF) solidification model, etc. Solution approximation error occurs when numerical solution techniques are employed to solve the mathematical model, such as discretization error, errors due to the use of reduced-order models, truncation error, etc. Additionally, surrogate model error is encountered when a surrogate model is used to approximate the expensive physics-based simulation model. Data uncertainty [31] is caused by sparse data (data generation is expensive), imprecise data (interval data), measurement error, qualitative data (expert opinion) etc. Aleatory uncertainty comes from the inherent variability in the process parameters across multiple builds or over time and space. The process parameter settings specified by the designer (such as the nozzle temperature, nozzle velocity, layer thickness, raster width, raster angle, etc.) may not be actually realized in manufacturing and may fluctuate due to variability in the equipment. Also, the model parameters discussed earlier may not be constant throughout the part, and may change spatially and also over time. These different sources of uncertainty need to be accounted for while optimizing the process design. Details of quantifying the above sources are provided in our previous work [32]; in this paper, we focus on quantifying the model discrepancy and including it in the process parameter optimization.

### 3.2.2. Model discrepancy quantification

Representing the AM simulation model as $G(d)$, the inputs $d$ can be divided into process parameters $X$ and model parameters $\theta$, i.e., $d = [X, \theta]$ where $X = [X_1, X_2, \ldots, X_{n_x}]$, $\theta = [\theta_1, \theta_2, \ldots, \theta_{n_\theta}]$, and $n_x$ and $n_\theta$ are the number of process parameters and model parameters respectively. The model output $y_m$ is given by

$$ y_m = G(X, \theta) \quad (13) $$

The surrogate model (discussed in Section 3.1.2) is trained with the data from the numerical model corrected for solution approximation error. The surrogate model error can be estimated by comparing the surrogate model prediction with numerical model output for another set of test data. The model form error (due to the assumptions and simplifications) causes discrepancy between the model prediction and experimental observation. In the Kennedy and O’Hagan (KOH) [33] framework, this model inadequacy is accounted for by using a model discrepancy
term $\delta$. When the errors are not quantified separately, the model discrepancy term includes the contribution of solution approximation errors as well. The relationship between model output and observation data ($y_{obs}$) is given by \[ y_{obs} = y_m + \delta - \epsilon_{obs} \] where $\epsilon_{obs}$ is the observation error in measurement.

Since $\delta$ and $\epsilon_{obs}$ are usually unknown, they need to be calibrated as well. $\epsilon_{obs}$ is commonly represented as a zero-mean Gaussian random variable with unknown variance $\sigma^2_{obs}$, i.e., $\epsilon_{obs} \sim N(0, \sigma^2_{obs})$. The model discrepancy may be a function of the input $X$ and can be formulated in various ways depending on the problem such as constant bias, random variable with fixed or input-dependent mean and variance, stationary or non-stationary Gaussian process [34]. Denoting the parameters of the model discrepancy function as $\Theta_{\delta}$, and when the model parameters are also considered uncertain, the calibration parameters $\Theta = [\theta, \theta_{\delta}, \sigma_{obs}]$. Using Bayes’ theorem, the joint posterior distribution of the calibration parameters is given by

$$ f(\Theta | y_{obs}) = \frac{f(y_{obs} | \Theta) f(\Theta)}{\int f(y_{obs} | \Theta) f(\Theta) d\Theta} $$

where $f(\Theta)$, $f(y_{obs} | \Theta)$, and $f(\Theta | y_{obs})$ are the joint probability density function (PDF) of $\Theta$, likelihood function, and the joint posterior PDF. This Bayesian calibration is generally performed using Markov Chain Monte Carlo (MCMC) sampling which requires repeated evaluation of the likelihood function to obtain the posterior distribution. Since the simulation models are prohibitively expensive, the surrogate model constructed earlier is used during model calibration.

### 3.2.3. FFF experiments and measurement

We conducted AM experiments in the laboratory to obtain data for validating the AM process models. The information collected is post-processed for fault diagnosis and comparison with numerical model prediction. Since some materials such as ABS (acrylonitrile butadiene styrene) have poor first layer adhesion and are prone to warping while printing, significant preparation of the printing environment is required to offset the challenges in printing quality parts. First, an enclosure is created (see Fig. 8) to thermally regulate the printing environment and prevent sudden temperature changes within the chamber. Second, the problem with first
layer adhesion of ABS with the build plate is solved by applying Kapton tape to the portion of the build surface where the specimen is to be printed. After these preparations, the quality of the FFF-produced part improved drastically as shown in Fig. 4. Use of laser-based sensors also introduces an additional challenge. If the printed parts are measured using a laser-based sensor, the laser beam must penetrate a non-transparent surface to serve as a baseline. Thus, the glass build plate is acid etched in its central region to provide an opaque surface for the optical displacement sensor to reliably operate. The measurement equipment and setup are determined depending on the QoI and the monitoring mode. The collected data during or after the printing is used for model validation as shown in Section 4.3.

![Figure 4: Comparison of FFF prints (a) before modifications, and (b) after modifications](image)

3.3. Optimization under uncertainty

A typical single-objective deterministic design optimization problem is formulated as follows:

\[
\begin{align*}
\min q(X) \\
\text{s.t.} \\
lb_{g_i} & \leq g_i(X) \leq ub_{g_i}, i = \{1, ..., n_g\} \\
lb_{X_j} & \leq X_j \leq ub_{X_j}, j = \{1, ..., n_X\}
\end{align*}
\]

where \(q(X)\) is the objective function to be minimized; \(X_j\) is the \(j\)-th design variable; \(g_i\) is the \(i\)-th design variable; \(n_X\) and \(n_g\) are the number of design variables and constraints, respectively; \(lb_{g_i}\) and \(ub_{g_i}\) are the lower and upper bounds of \(g_i\); \(lb_{X_j}\) and \(ub_{X_j}\) are the lower and upper bounds of \(X_j\).

In the AM process design optimization, the objective function can be related to geometric accuracy of the part, porosity, mechanical properties, material and energy consumption, cost
of production, etc. The objective function depends on the intended use of the part. In some cases, multi-objective formulations may be necessary; the objectives may either conflict with or support each other. For example, it has been reported that dimensional accuracy, surface quality, and filament bonding do not all achieve their best values simultaneously for the same process parameter values \[35\]. On the other hand, minimizing porosity increases the part’s strength \[35\].

The multiple objectives can be handled by combining the objectives using a weighted sum method. The objective function is rewritten as follows:

\[
\min q = (w_1 q_1(X) + w_2 q_2(X)) 
\]  

(17)

where weights \(w_1\) and \(w_2\) express relative preferences among the objectives \(q_1\) and \(q_2\) respectively and \(w_1 + w_2 = 1\).

However, the major challenge in the optimization of the AM process is the uncertainty in the process and its modeling. As discussed in Section 3.2, the various sources of uncertainty lead to uncertainty in the prediction of the QoI. Thus, the objective function and the constraints in Eq. 16 may not be deterministic. Optimization under uncertainty can be handled by two types of formulations: (a) reliability-based design optimization (RBDO), and (b) robust design optimization (RDO). In RBDO, the objective function is optimized while ensuring that the reliability is above a desired threshold \[36\]. Whereas, in RDO, either the objective function or the constraints, or both, are required to be within specified bounds \[37\]. In this work, the RDO formulation is used, and we consider the mean and variance of part thickness. Thus RDO can be represented as a multi-objective optimization problem with two objectives: (a) Optimize the mean of the part thickness, and (b) Minimize the variance of the part thickness \[37\]. This multi-objective optimization is converted to a single objective optimization formulation similar to Eq. 17

\[
\min q = (w_1 \mu_q(X) + w_2 \sigma_q(X)) 
\]  

(18)

where \(\mu_q\) and \(\sigma_q\) are the mean and standard deviation respectively of \(q\). When the constraint is also stochastic, the feasible region is reduced to satisfy the constraints in the presence of uncertainty \[38\]. The width of the feasible region is reduced by \(k_c \sigma_q\) in each direction; where \(k_c\) is a user-defined constant depending on the design requirements and \(\sigma_q\) is the standard deviation.
of the constraint [37, 38]. The constraints can be written as:

\[ lb_i + k_c \sigma_g(g_i(X)) \leq g_i(X) \leq ub_i - k_c \sigma_g(g_i(X)), \quad i = \{1, \ldots, n_g\} \]

(19)

For a given \( X \), representing \( f_q^x(q) \) as the probability density function (PDF), we have

\[ \mu_q(X) = \int_{-\infty}^{\infty} q f_q^x(q) \, dq \]

(20)

\[ \sigma_q^2(X) = \int_{-\infty}^{\infty} (q - \mu_q)^2 f_q^x(q) \, dq \]

(21)

After further simplifications and using Monte Carlo simulation (MCS) for integration, the above equations can be approximated as follows [19]:

\[ \mu_q(X) \simeq \frac{1}{n_m} \sum_{i=1}^{n_m} m_1^i(X, \Theta_i) \]

(22)

\[ \sigma_q^2(X) \simeq \frac{1}{n_m} \sum_{i=1}^{n_m} m_2^i(X, \Theta_i) - \left( \frac{1}{n_m} \sum_{i=1}^{n_m} m_1^i(X, \Theta_i) \right)^2 \]

(23)

where the conditional PDF \( f_q^x(q | \Theta) \) depends on the values of the parameters \( \Theta \) defined in Eq. 15, \( m_1^i(X, \Theta_i) = \int_{-\infty}^{\infty} q f_q^x(q | \Theta_i) \, dq \) and \( m_2^i(X, \Theta_i) = \int_{-\infty}^{\infty} q^2 f_q^x(q | \Theta_i) \, dq \) are the mean and second moment of \( q \) respectively for given \( X \) and the \( i \)-th MCS sample of \( \Theta \). The objective function is now given by substituting Eqs. 22 & 23 in Eq. 18. The RDO formulation is as follows:

\[
\min \left[ w_1 \left( \frac{1}{n_m} \sum_{i=1}^{n_m} m_1^i(X, \Theta_i) \right) + w_2 \left( \frac{1}{n_m} \sum_{i=1}^{n_m} m_2^i(X, \Theta_i) - \left( \frac{1}{n_m} \sum_{i=1}^{n_m} m_1^i(X, \Theta_i) \right)^2 \right) \right]
\]

s.t.

\[ lb_i + k_c \sigma_g(g_i(X)) \leq g_i(X) \leq ub_i - k_c \sigma_g(g_i(X)), \quad i = \{1, \ldots, n_g\} \]

\[ lb_{X_j} \leq X_j \leq ub_{X_j}, \quad j = \{1, \ldots, n_X\} \]

\[ w_1 + w_2 = 1 \]

(24)

Since the objective function needs to be evaluated repeatedly, the surrogate model constructed previously in Section 3.1.2 is used for faster computation. The design variables in the AM process are the controllable process parameters. As discussed in Section 1, several studies have investigated the effects of process parameters on the part’s performance and quality. Some
of the process parameters such as layer thickness are discrete, whereas extrusion temperature and extrusion velocity are continuous variables. The constraints in the optimization problem could be from considerations such as the print time for the part to be within a reasonable value; other constraints may be due to the limitations of the printer such as the maximum extrusion volume of the nozzle, minimum allowable layer thickness, etc. In the case of stochastic constraints given by Eq. 19, the standard deviations of the constraints can be estimated by using a first-order Taylor series approximation, Monte Carlo simulation (MCS), etc. [39]

Depending on the design variables and the constraints, the optimization problem defined in Eq. 24 can be solved by using a suitable global optimization algorithm. For optimization problems with a smaller feasible space due to lesser number of design variables with small ranges, a brute-force optimization technique may be adequate. However, when the entire design space cannot be as easily explored, metaheuristic techniques such as simulated annealing (SA), genetic algorithm (GA), particle swarm (PS), etc. can be employed to approximate the global optimum solution $X_{opt}$. SA is generally used for a discrete search space [40], whereas for unconstrained nonlinear optimization problems with continuous variables, PS is more efficient than GA [41]. Other optimization techniques such as grid search, trajectory methods, clustering methods, etc. [42] can also be used. The formulation presented above for AM process parameter design is valid irrespective of the algorithm chosen to solve the optimization problem.

### 3.4. Summary

The steps of proposed framework for AM process parameter design under uncertainty can be summarized as follows:

Step 1: Development of physics-based AM simulation models.

Step 2: Analysis of the uncertainty sources.

Step 3: Correction of the AM model for numerical solution error.

Step 4: Construction of surrogate model to replace the expensive simulation model.

Step 5: Collection of experimental data for model calibration.

Step 6: Calibration of the uncertain model parameters and model discrepancy using experimental data.

Step 7: Aggregation of uncertainty from the calibration results.
Step 8: Formulation and solution of the optimization problem using the calibrated model.

The methodology presented in this paper can be generalized for any AM process (with corresponding physics models and experiments). For a new part geometry or a different AM process, a new surrogate model needs to be constructed using the physics model runs and then corrected using experimental data. Even this additional effort still results in material and energy savings compared to the trial-and-error approach. The savings are even more prominent for metal parts that are much more expensive to produce than polymer parts. In the next section, we demonstrate the proposed methodology with an illustrative example.

4. Illustrative example

Consider a part of dimensions 35 mm $\times$ 12 mm $\times$ 4.2 mm printed with ABS. The material parameters used in this example, given in Table 3, are considered to be known or previously estimated. In this example, the aim is to optimize the process parameters: extrusion temperature ($T_e$), extrusion velocity ($V_e$), and layer thickness ($l_t$) i.e, $X = [T_e, V_e, l_t]$ for three different cases described in Section 4.5. Considering the limitations of the printing machine and the available computational resources, the process design variables are assumed as shown in Table 2. Following the procedure summarized in Section 3.4, the proposed methodology is demonstrated in this section.

Table 2: Process parameter range

<table>
<thead>
<tr>
<th>Process parameter</th>
<th>Variable type</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_e$</td>
<td>Integer</td>
<td>215$^\circ$C to 280$^\circ$C</td>
</tr>
<tr>
<td>$V_e$</td>
<td>Integer</td>
<td>25 mm/s to 45 mm/s</td>
</tr>
<tr>
<td>$l_t$</td>
<td>Discrete</td>
<td>0.42 mm, 0.6 mm, 0.7 mm</td>
</tr>
</tbody>
</table>

4.1. FFF simulation

A finite element model of the part is first created using the commercial software Abaqus as shown in Fig. 5. The extrusion of the material is approximated by element deactivation-activation. As described in 3.1.1, activation by raster line is used for this example. The elements for the raster line, initially all deactivated, are activated one after the other in subsequent time steps to mimic the extrusion process.
4.1.1. Heat transfer simulation

For heat transfer analysis, the build plate temperature of 110 °C is considered as a boundary condition for the layers in contact with the build plate. Heat loss due to convection and radiation is considered during the process. The extrusion temperature $T_e$ is applied as a pre-defined temperature field to the elements. Fig. 5 shows the mesh consisting of 8-noded linear heat transfer brick elements DC3D8. The output temperature field as a function of time is then exported to the mechanical model.

Table 3: Material properties of ABS [6]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal conductivity</td>
<td>0.15 W/°C m</td>
</tr>
<tr>
<td>Specific heat</td>
<td>1290 J/°C Kg</td>
</tr>
<tr>
<td>Thermal expansion coefficient</td>
<td>$9 \times 10^{-5}$</td>
</tr>
<tr>
<td>Density</td>
<td>4428 kg/m³</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>1826 MPa</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.32</td>
</tr>
<tr>
<td>Yield strength</td>
<td>25 MPa</td>
</tr>
</tbody>
</table>

4.1.2. Structural deformation simulation

The mechanical model has the same geometry and mesh as the thermal model. The temperature field obtained from the heat transfer model is applied as thermal loading in this model. The base of the part is assumed to be fixed with the build plate. In the Abaqus implementation, 8-noded linear 3D stress brick element C3D8 is used. The temperature field from the heat transfer analysis and the deformation in the z-direction from the structural deformation analysis after the final raster line is laid are shown in Fig. 6. The average thickness $t$ of the part is computed from the deformation field obtained from the structural analysis simulation, which is the QoI in this example, i.e., $y_m = t$.

The FE analysis were performed on Intel® Core™ i7-4790 CPU@3.60 GHz, 16GB RAM with 4 CPUs. Depending on the process parameter values, the thermal model required between
15 minutes and 4 hours to complete the simulation, and the mechanical model required between 30 minutes and 8 hours.

4.2. Surrogate model

As mentioned in Section 3, UQ analysis and optimization require multiple evaluations of the model. Thus, the two FE models described in Section 4.1 are together replaced by a GP surrogate model. To construct the surrogate model, 25 samples of the process parameters as shown in Fig. 7 are generated using the Latin hypercube sampling (LHS) technique for design of experiments, i.e., \( X^s_i = [T_{ei}, V_{ei}, l_{ti}], \forall i = 1, 2, \ldots, 25 \) from the feasible range of the optimization decision variables (process parameters) given in Table 2. For each of these 25 samples, FE analysis are carried out, and the average thickness \( y_{mi}^s = t_{si}^l \), \( \forall i = 1, 2, \ldots, 25 \) of the manufactured part is predicted. A GP model is created with the process parameters \( X^s \) as inputs and the predicted average thickness \( y_{mi}^s \) of the part as output. The quality of the surrogate model constructed is evaluated using LOOCV discussed in Section 3.1.2. The surrogate model error (i.e., difference between the FE model prediction and the mean prediction of the surrogate model) was found to be less than 7% (MAPE LOOCV value), which is assumed to be adequate in this example; the accuracy can be further increased by using additional training samples. In the case of a more complicated part with a larger number of process parameters, more samples will be required for training the surrogate model. The run time for the FE model also increases as the number of nodes increases for a complicated part. However, adaptive mesh refinement techniques and commercial FE analysis software with sophisticated AM analysis capabilities can be used to reduce the run time. High performance computing can also be utilized if available. As discussed in Section 3.1.2, adaptive training approaches may be considered for efficient surrogate model construction to further reduce the computation expense.
4.3. Experimental data

Experiments are conducted to validate the predicted average thickness of the part. The raster width and raster angle are kept constant for the experiments whereas the layer thickness is varied since it is a design variable. The parts are printed using Ultimaker S5 [43] 3D printer and the part thickness is measured offline with a laser displacement sensor Keyence LK-H057 [44] (Fig. 8).

![Experimental setup for FFF: (a) 3D printer, (b) laser displacement sensor](image)

Figure 8: Experimental setup for FFF: (a) 3D printer, (b) laser displacement sensor

The optical displacement sensor Keyence LK-H057 (accuracy of ±0.02% and repeatability of 0.01μm) [44] gives the thickness at a point location. The instrument was checked by measuring a standard calibration block. Repeated measurements of the calibration block were correct, and
consistent within 0.01µm. This accuracy is sufficient to capture thickness variation since we are working with thickness of the order of 0.1µm. The analysis in this paper requires measuring the part thickness at multiple locations. The displacement sensor is fitted on a linear rail, and actuated along its axis over the specimen in a forward/backward motion to collect data at cross-section locations 7, 12, 17, 22, and 27 mm of the part along the length as can be seen in Fig. 9. The average thickness of the part is calculated from the collected field data. The initial setup of the printer along with leveling of the build plate takes around 20 minutes. Subsequently, for the experiments including printing of the part and collecting part thickness data using the displacement sensor requires 10 minutes on an average.

![Figure 9: Cross-section for part thickness measurement](image)

4.4. Integration of model prediction and experimental data

The next step is to integrate the prediction from the FFF simulation model in Section 4.1 and the data collected from experiments in Section 4.3 to perform model calibration. The observation data of part thickness is collected for three sets of process parameters i.e., \( \mathbf{y}^{\text{obs}} = [y_1^{\text{obs}}, y_2^{\text{obs}}, y_3^{\text{obs}}] \) where \( y_j^{\text{obs}}(\mathbf{X}_j^{\text{obs}}), \forall j = 1, 2, 3 \) is the observation at process parameter setting \( \mathbf{X}_j^{\text{obs}} \). At each setting, three copies of parts are printed and their thickness measured. The observation error is estimated from the experimental data and hence is considered known. Thus the only quantity to be calibrated is the model discrepancy term. Note that since the discretization error is not estimated separately, the model discrepancy term also includes the discretization error.

Since a limited number of observation data are available, the model discrepancy term \( \delta \) is modeled here as a Gaussian random variable with unknown mean and standard deviation \( \mu_d \) and \( \sigma_d \) respectively, i.e., \( \delta \sim N(\mu_d, \sigma_d) \). Thus, the calibration quantities are \( \Theta = [\mu_d, \sigma_d] \). The model discrepancy term, in this case, is represented as independent of the input. Input-
dependent formulations for model discrepancy, discussed in Section 3.2.2, have more parameters and can be considered when sufficient data is available for the estimation of model discrepancy parameters. The prior distributions of the parameters $\Theta$ are assumed to be uniform (Table 4). Using the data $y^{obs}$ in Eq. 15, the calibration of parameters of the discrepancy term (referred to as hyper-parameters) is performed. The posterior distributions shown in Fig. 10 indicate the reduction of uncertainty in comparison to the prior distributions. The uncertainty in the prediction can be further reduced by performing calibration using additional experimental data. More comprehensive modeling of the discrepancy term can also be pursued as mentioned in Section 3.2.2. Note that in the case when a higher fidelity model is used to simulate the AM process, the calibrated value of the model discrepancy would be lower indicating that the model is more accurate and closer to the physical system being simulated. The proposed optimization methodology can be implemented with any physics-based model, as long as the model error is included in UQ, and when the model error is acceptably small.

Table 4: Prior distribution of the calibration parameters

<table>
<thead>
<tr>
<th>Variable</th>
<th>Distribution</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_d$</td>
<td>Uniform</td>
<td>[-1,0.5]</td>
</tr>
<tr>
<td>$\sigma_d$</td>
<td>Uniform</td>
<td>[0,1]</td>
</tr>
</tbody>
</table>

Figure 10: Calibration of hyper-parameters of model discrepancy: (a) mean and (b) standard deviation

In the forward uncertainty propagation, the model discrepancy term is simulated using Monte Carlo samples from the posterior distributions of the hyper-parameters. The model discrepancy term is added to the surrogate model prediction to obtain the corrected model prediction, which is then used in the process parameter optimization in the next subsection. Using the thermo-mechanical model described in Section 3.1 once the model discrepancy is quantified and added to the model prediction, Fig. 11 shows that the experimental observation falls
within half the standard deviation of the corrected model prediction. Thus, since optimization under uncertainty requires many physics model runs, a practically feasible approach is to use a corrected lower fidelity model for optimization purposes, and then use the more sophisticated model for accurate prediction for a specific solution.

![Figure 11: Comparison of corrected physics model prediction and observation from physical experiments](image)

4.5. Process parameter optimization

This subsection presents the results of process parameter optimization. The surrogate model constructed in Section 4.2 and corrected with the model discrepancy term calibrated in Section 4.4 is now utilized to find the optimal process parameters in the following cases.

**Case 1**

Geometric accuracy of the part produced by the FFF process is an important consideration. For the manufactured part to be useful, the difference between the target geometry and the manufactured geometry should be minimal. In this case, the objective is to determine the optimal process parameters that minimize the thickness error, i.e., the difference between the target thickness of 4.2 mm and the predicted average thickness of the manufactured part. The design variables are \( \mathbf{X} = [T_c, V_e, l_t] \). The bounds of the design variables are given in Table 2. For the experimental setup used in Section 4.3, the maximum extrusion volume [43] for the 0.8 mm diameter nozzle used in the experiments is 24 mm\(^3\)/s. This limitation adds a constraint to the optimization problem. The maximum extrusion volume constraint is given by

\[
V_e \times l_t \times L_w \leq 24
\]  

(25)
where $L_w$ is the raster width fixed at 0.8 mm. This is a deterministic constraint since the design variables and raster width are considered deterministic.

First only the mean prediction of the thickness error is considered i.e., $w_1 = 1$ and $w_2 = 0$ in Eq. 24. Given the small feasible region in this example due to a small number of possible discrete values of the optimization variables, an exhaustive search is used to find the optimal solution. The optimal solution is found to be $[T_e = 231^\circ C, V_e = 43 mm/s, l_t = 0.42 mm]$. In this case, the least layer thickness (0.42 mm) is the optimal solution as expected. To validate the optimization result, parts are printed and measured at five other process parameter settings selected at random and compared to the part printed with the optimal solution. It is found that at all the other settings, the mean thickness error is more than that of the optimal solution (Fig. 12).

As discussed in Section 3.3, in order to achieve parts with consistently good quality, it is important to consider the prediction variance as well. Assuming that equal weight is assigned to minimizing mean thickness error and minimizing standard deviation of predicted thickness error, $w_1 = w_2 = 0.5$. The optimal solution is $[T_e = 231^\circ C, V_e = 43 mm/s, l_t = 0.42 mm]$, which is the same as $w_2 = 0$ scenario. However, when only standard deviation of predicted thickness error is considered, i.e., $w_1 = 0$ and $w_2 = 1$, the optimal solution is $[T_e = 248^\circ C, V_e = 35 mm/s, l_t = 0.7 mm]$. This implies that prediction variance has a lower contribution.

<table>
<thead>
<tr>
<th>Process parameter setting</th>
<th>Mean thickness error (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.05</td>
</tr>
<tr>
<td>0.05</td>
<td>0.1</td>
</tr>
<tr>
<td>0.1</td>
<td>0.15</td>
</tr>
<tr>
<td>0.15</td>
<td>0.2</td>
</tr>
<tr>
<td>0.2</td>
<td>0.25</td>
</tr>
<tr>
<td>0.25</td>
<td>0.3</td>
</tr>
<tr>
<td>0.3</td>
<td>0.35</td>
</tr>
<tr>
<td>0.35</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Figure 12: Experimental validation of optimal process design
than prediction bias to the weighted objective function. The variance in the prediction is due to the variance of the surrogate model prediction and the variance of the model discrepancy term. The variance in the prediction is due to the variance of the surrogate model prediction and the variance of the model discrepancy term. Since the surrogate model prediction variance is negligible (less than 1% of the mean surrogate model prediction), the variance in the prediction mostly comes from the model discrepancy term. As mentioned earlier (Section 4.4), in this example the model discrepancy has been estimated with only three observation data. With more data, the model discrepancy may be modeled as a function of the process parameters, thus allowing for investigation of the effects of the process parameters on the uncertainty due to model discrepancy. Such investigation, through variance-based global sensitivity analysis [45], would also be able to identify process parameters that have a dominant effect on the model discrepancy, and guide the representation of model discrepancy as a function of the dominant process parameters.

Case 2

It is observed in the previous case that the optimal solution for mean thickness error is achieved with the smallest layer thickness. This is generally expected in AM process. To verify this, the mean thickness error at random process parameter settings was predicted using the corrected surrogate and similar trends were observed. In Fig. 13, the predicted mean thickness error at random process parameter settings is plotted against the layer thickness. It can be seen that mean thickness error has smaller values for the least layer thickness of 0.42 mm, followed by 0.6 mm layer thickness.

However, when manufacturing larger parts there might be an additional constraint of print time (which is affected by layer thickness; smaller layer thickness will cause longer print time for the entire part). High print time for batch production of parts may be unaffordable. In such cases, the optimization problem is illustrated here with two competing objectives: minimizing the mean thickness error and minimizing the print time. The design variables, variable bounds, and constraints are the same as the Case 1. In this case, instead of just optimizing the objective function for equal weights, a Pareto front Fig. 14 is obtained by varying the weights from 0 to 1 in increments of 0.1. In Fig. 14, the point A corresponds to the case when the objective is to minimize mean thickness error irrespective of the print time; and point D is obtained when the objective is to minimize print time without any restriction on the mean thickness error.
The points between $A$ and $D$ consider non-zero weights for both the objectives. The process parameter settings for these points in the Pareto front are given in Table 5. (Note that 11 values of weights were considered, from 0 to 1 in increments of 0.1; the solutions for several weight combinations coincided with each other, thus the interior points on the Pareto curve represent solutions for multiple weight combinations).

The optimization results from the Pareto chart obtained using the model-based approach for process parameter optimization are validated by printing and measuring the parts corresponding to the points $A, B, C,$ and $D$ of the Pareto chart. The experimental observations of the mean thickness errors corresponding to the Pareto chart points are listed in Table 5. It is seen in Fig. 14 that the smaller layer thickness gives better quality in terms of mean thickness error (point $A$) whereas the largest layer thickness takes lesser time to print (point $D$) but has high thickness error. The corresponding mean thickness error measurements of the printed parts for points $A$ and $D$ show the same result. Points $B$ and $C$ are expected to have mean thickness error between the two extreme points ($A$ and $D$). The measured values for these points also agree with this expectation. Thus, the effectiveness of the proposed process optimization framework has been demonstrated with physical experiments.
5. Conclusion

In this paper, a physics model-based approach, enhanced with experimental data, is proposed for the design optimization of process parameters in AM, and the proposed approach is illustrated for the FFF process. The main components of the proposed framework are the development of physics-based models for the FFF process, UQ analysis by integrating the models and experiments, and design optimization under uncertainty. A surrogate model is built to substitute the expensive physics-based AM models for faster UQ analysis. AM experiments conducted in the laboratory are used to correct the numerical model by calibrating the model discrepancy term. This corrected model is used for process design optimization under uncertainty with respect to geometric inaccuracy, considering the cases: minimize the mean of thickness error, minimize the variance of thickness error, minimize the mean and variance of thickness error,
and minimize the mean thickness error and printing time. The results of the optimization are validated with experimental results.

Future efforts can consider implementing the proposed framework with a larger number of process parameters and including aleatory variability in the process parameters. The latter is caused when the parameter settings specified by the designer are not achieved in the system, or when the process parameters fluctuate during printing. The current work also lays the foundation for process control in AM. When in situ measurements (online monitoring) of part thickness are available after every layer during the manufacturing process, the developed framework can be extended to control the process parameters in a layer-wise fashion to minimize the variability in part quality.

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References


