Inverse and forward sparse-grids-based uncertainty quantification analysis of laser-based powder bed fusion of metals

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Abstract

The present paper aims at applying uncertainty quantification methodologies to process simulations of Laser-based Powder Bed Fusion of Metals. In particular, for a part-scale thermomechanical model of an Inconel 625 super-alloy beam, we study the uncertainties of three process parameters, namely the activation temperature, the powder convection coefficient and the gas convection coefficient. First, we perform a variance-based Global Sensitivity Analysis to study how each uncertain parameter contributes to the variability of the beam displacements. The results allow us to conclude that the gas convection coefficient has little impact and can therefore be fixed to a constant value for subsequent studies. Then, we conduct an inverse uncertainty quantification analysis, based on a Bayesian approach on synthetic displacements data, to quantify the uncertainties of the activation temperature and the powder convection coefficient. Finally, we use the results of the inverse uncertainty quantification analysis to perform a data-informed forward uncertainty quantification analysis of the residual strains. Crucially, we make use of surrogate models based on sparse grids to reduce the computational burden.

Keywords: Additive Manufacturing, Uncertainty Quantification, Bayesian inversion, Sparse Grid.

1. Introduction

Additive Manufacturing (AM) \[1\] is a technology that is able to produce components with complex geometries and high mechanical performances by means of a layer-by-layer strategy. Among the different AM technologies available for the production of metallic components, Laser-based Powder Bed Fusion of Metals (PBF-LB/M) is nowadays the most widespread \[2, 3\]. PBF-LB/M processes start by distributing a layer of metal powder particles on a build plate within a closed chamber where an inert gas (argon or nitrogen) is inflated. The metal powder is then selectively melted by means of a high-energy-density laser source following a predefined scan path. Once the layer scan is completed, a new layer of metal powder is deposited on top of the previous one by means of a roller and the process is repeated until the final component is terminated.

Due to the multi-scale and multi-physics nature of the process, complex process-structure-property relationships occurring in PBF-LB/M processes are not fully understood yet \[4\]; thus, proper calibration of a large set of parameters still requires long and expensive trial-and-error experimental approaches. To this end, computer-aided simulations of the PBF-LB/M process can play a crucial role in the AM production of metallic components \[5\]. In the literature, we can find a large set of numerical models suitable for AM simulations, which can be classified into three main classes based on their reference length scale, namely: micro, meso, and macro-scale \[6\]. Micro-scale models, also called powder-scale models, provide information on the effect of the laser beam on the microstructure evolution and grain structure; they are typically solved using, e.g., Phase-Field methods \[7, 8\] or Cellular Automata \[9\]. Meso-scale models investigate the effect of the scanning strategy and the laser parameters on melt-pool dynamics and are typically solved using e.g., the Lattice-Boltzmann method \[10\] and the Discrete Element method \[11\]. Finally, macro-scale models, also called part-scale models, allow the prediction of the mechanical response of the component, including the study of quantities such as residual stresses and thermal distortions at part-scale. The most popular method in part-scale AM numerical analysis is the Finite Element (FE) method \[12–14\].
PBF-LB/M processes include several sources of uncertainty, due to the inherent variability of the process parameters [15–17], e.g., powder particle radius, mechanical properties of powder particles, physical-chemical properties of the material. Uncertainty Quantification (UQ) methodologies are a suitable tool to quantify and reduce the influence of such uncertainties on both the process and product quality [18, 19]. In particular, forward UQ analysis studies the propagation of uncertainties from the parameters – modeled as random variables with uncertainty described by the associated probability density function (PDF) – to the outputs of the model, also called Quantities of Interest (QoIs) of the problem. On the contrary, inverse UQ analysis aims at reducing the uncertainty on the model parameters, estimating the plausibility of the different possible values that the parameters can take given a set of experimental data, using, e.g., Bayesian inversion techniques [20–22]. Therefore, inverse UQ analysis can be seen as closely related to parameter calibration, but – instead of providing a specific value for the calibrated parameters – it returns a “data-informed” PDF.

The effectiveness of UQ techniques for AM processes is widely recognized for applications in production-level experiments, whereas their application to AM simulations (e.g., for validation of computational models) still remains an open challenge. A wider adoption of UQ techniques in AM simulations is hindered by the difficulty of quantifying uncertainties on both model input parameters and computational models (e.g., uncertainties due to the mathematical simplifications introduced for the physical representation of the AM process and the approximations introduced to implement the algorithms). Therefore, most of the works on UQ for AM simulations present in the literature are limited to a forward UQ analysis, investigating the propagation of the process parameter uncertainties on the QoIs. In this framework, Lopez et al. [16] presented a discussion on the origin and propagation of uncertainty in PBF-LB/M models. Mahmoudi [23] developed a design of experiments approach to study the effects of uncertainties due to PBF-LB/M input parameters. Grasso and Colosimo [24] developed a method based on principal component analysis for spatial identification of defects during the PBF-LB/M process. However, the interest in inverse UQ techniques is rapidly growing. In fact, the capability of this method to quantify uncertainties on input parameters would dramatically increase the reliability of simulated results. Accordingly, Nath et al. [17] proposed a framework for modeling and quantifying the uncertainty of material properties. Korshunova et al. [25] introduced a random field model in combination with the Finite Cell Method to efficiently evaluate the influence of microstructure on the variability of the mechanical behavior of AM products.

Another critical problem hampering the application of UQ techniques for computational AM models is the large number of simulations required and the high computational cost associated to a single thermomechanical analysis. To reduce this computational burden, a viable approach is to replace the results of the full AM model with cheaper evaluations of so-called surrogate models. Surrogate models are obtained by first running a limited number of full model simulations; these full model results are then, e.g., interpolated or approximated by least-squares to create a response surface to, finally, compute inexpensive problem solutions avoiding full model, computationally demanding runs. Therefore, surrogate modeling approaches can be considered the key to overcome the computational burden affecting UQ technology. In the literature, most of the surrogate models suitable for UQ of AM processes are based on Gaussian processes and focus on experimental melt-pool parameters. Xie et al. [26] quantified model, code, and data uncertainties in a melt-pool model using measurement data on melt pool geometry (length and depth). Wang et al. [27] proposed a sequential Bayesian calibration method to perform calibration of experimental parameters and model correction to significantly improve the validity of the melt-pool surrogate model. Nath et al. [28] presented an inverse UQ framework predicting the microstructure evolution during solidification by coupling a surrogate meso-scale melt-pool model with a micro-scale cellular automata model.

In the present paper, we propose and apply a UQ approach to quantify the uncertainties involved in the simulation of a PBF-LB/M process using a part-scale thermomechanical model of an Inconel 625 beam (i.e., at a different scale compared to the above-mentioned contributions [26–28]). In particular, we want to study the influence of the activation temperature, the powder convection coefficient and the gas convection coefficient in order to obtain reliable residual strains in a PBF-LB/M produced part. We remark that the part-scale thermomechanical model considered in the present work highly simplifies the physics of the process and therefore the parameters that we consider are in a way only conceptual (i.e., they cannot be directly measured in reality): for this reason an inverse UQ analysis is mandatory to suitably define their ranges and PDFs. Conversely, the UQ analysis in [26–28] focuses on melt pool model parameters, that can actually be measured (either directly or indirectly) to obtain a prior PDF that is at least partially consistent with reality. Moreover, our approach is not based on mechanical responses obtained by experiments but rather by part-scale thermomechanical numerical simulations: this allows us to remove any errors due
Figure 1: AM model of a cantilever beam 75 mm long, 12 mm high and 5 mm wide with a build plate measuring 85 mm long, 12 mm high and 20 mm wide. Points marked in blue numbers and orange letters will be used during the UQ analysis; the green dotted line marks the location where we will compute residual strains; the red contours indicate the removal area.

to the inherent mismatch between reality and our part-scale thermomechanical model; consequently, any error/sub-optimal result (either in the calibration or in the subsequent forward uncertainty propagation) can be attributed solely to the adopted methodology. A further difference between the present work and [26–28] is that in our work we use a different surrogate modeling methodology, namely sparse-grid surrogate models [29–31] (using the Sparse-Grids Matlab kit [32] implementation) instead of Gaussian process regression. The results show that sparse grids are indeed very effective in reducing the number of full model analyses needed (and thus the overall computational cost of the proposed approach), but a comparison between Gaussian processes and sparse grids is not provided here since it exceeds the scope of the current work.

The present work is structured as follows. In Section 2, we present the part-scale thermomechanical model to describe PBF-LB/M process simulation. In Section 3, we describe the developed UQ approaches, both forward and inverse. In Section 4, UQ results are reported and discussed. Finally, in Section 5, we draw the main conclusions and possible further perspectives of the present work. We also report some technical background information in Appendix A and Appendix B.

2. Part-scale thermomechanical model

In the present work, we employ a part-scale thermomechanical model [12–14] to simulate the PBF-LB/M process of an Inconel 625 beam (Figure 1) according to the design experiment proposed by the National Institute of Standards and Technology (see [33] for more details on component geometry). In Section 2.1 we introduce the governing equations that describe the thermal and mechanical problems involved in the PBF-LB/M process, whereas in Section 2.2, we present the numerical approach used to simulate the process.

2.1. Governing equations

2.1.1. Thermal problem

Assuming that the material follows Fourier’s law, the thermal problem is governed by the temperature-based heat transfer equation as follows [34]:

$$\rho c_p(T) \frac{\partial T}{\partial t} - \nabla \cdot (k(T) \nabla T) = 0 \quad \text{in} \quad \Omega,$$

where $T$ is the temperature field, $\rho$ denotes the constant material density, $c_p$ is the temperature-dependent specific heat capacity at constant pressure, and $k$ is the temperature-dependent thermal conductivity.

The thermal problem initial condition at time $t = 0$ is set as

$$T = T_0 \quad \text{in} \quad \Omega,$$
whereas the Dirichlet and the Neumann boundary conditions on domain’s boundary, \( \partial \Omega = \partial \Omega_Q \cup \partial \Omega_T \cup \partial \Omega_H \), are defined as follows:

\[
T = \bar{T} \quad \text{on} \quad \partial \Omega_T \subset \partial \Omega, \\
k \nabla T \cdot n = \bar{q} \quad \text{on} \quad \partial \Omega_Q \subset \partial \Omega,
\]

where \( \bar{T} \) is the temperature of the environment on the build plate lateral surface boundary \( \partial \Omega_T \), and \( \bar{q} \) denotes the heat loss through the free surface of normal \( n \) on the boundary lateral and upper surface of the beam \( \partial \Omega_Q \); on the remaining portion of the domain boundaries \( \partial \Omega_H \) adiabatic conditions are imposed.

In the PBF-LB/M simulation process at part-scale, the heat loss through the boundary can be described by means of two heat transfer mechanisms: heat loss by conduction through the powder, denoted by \( q_p \), and heat loss by convection through the environment gas, denoted by \( q_g \). Therefore, the heat loss \( \bar{q} \) is split into two terms as follows:

\[
\bar{q} = q_p + q_g.
\]

Since powder is not included in our model, both heat loss mechanisms can be modeled by means of two convection-like boundary conditions by means of two different heat transfer coefficients: a powder convection coefficient, \( h_p \), and a gas convection coefficient, \( h_g \), respectively. Therefore, following Newton’s law, we can formulate the two different heat loss terms as:

\[
q_p = h_p(T - \bar{T}) \quad \text{on} \quad \Gamma_p \subset \partial \Omega_Q, \\
q_g = h_g(T - \bar{T}) \quad \text{on} \quad \Gamma_g \subset \partial \Omega_Q,
\]

where \( \Gamma_p \) and \( \Gamma_g \) are the powder-component interface and the environment-gas-component interface, respectively, with \( \partial \Omega_Q = \Gamma_p \cup \Gamma_g \) and \( \Gamma_p \cap \Gamma_g = \emptyset \).

### 2.1.2. Mechanical problem

The solution of the mechanical problem is given by solving the equilibrium equation:

\[
\nabla \cdot \sigma = 0 \quad \text{in} \quad \Omega,
\]

with \( \sigma \) the Cauchy stress tensor defined as:

\[
\sigma = D^{el} \varepsilon^{el},
\]

where \( D^{el} \) is the isotropic elasticity tensor, depending on the Young’s modulus of elasticity and Poisson’s ratio, and \( \varepsilon^{el} \) is the elastic strain. The total strain in the material, \( \varepsilon^{tot} \), can be decomposed into elastic strain, \( \varepsilon^{el} \), thermal strain, \( \varepsilon^{th} \), and plastic strain, \( \varepsilon^{pl} \), as:

\[
\varepsilon^{tot} = \varepsilon^{el} + \varepsilon^{th} + \varepsilon^{pl} = \frac{1}{2} [\nabla u + (\nabla u)^T],
\]

with \( u \) the displacement vector.

In our thermomechanical model, the thermal strain acts as an external (thermal) load and is defined as follows:

\[
\varepsilon^{th} = \alpha \Delta T \mathbf{I},
\]

with \( \alpha = \alpha(T) \) the temperature-dependent thermal expansion coefficient, \( \Delta T \) the variation in time of the temperature field, and \( \mathbf{I} \) the second-order identity tensor.

Finally, the plastic strain rate \( \dot{\varepsilon}^{pl} \) is computed following the Prandtl-Reuss flow rule [12, 35, 36] as follows:

\[
\dot{\varepsilon}^{pl} = \frac{\gamma}{\Delta \sigma} \frac{\partial \Sigma}{\partial \sigma}
\]

where \( \gamma \) is the equivalent plastic strain, \( \Sigma = \sigma_{\text{von}} - \sigma_y \leq 0 \) is the yield function describing the material through the equivalent Von Mises stress, \( \sigma_{\text{von}} = \sqrt{\frac{1}{2} \mathbf{s} : \mathbf{s}} \) with \( \mathbf{s} = \sigma - tr(\sigma) \mathbf{I} \), and the temperature-dependent yield stress,
\( \sigma_y = \sigma_y(T) \) [12, 35, 36].

The mechanical problem is solved with the following Dirichlet boundary condition:

\[
u = 0 \quad \text{on} \quad \partial \Omega \cap \partial \Omega_U,
\]

with \( \partial \Omega_U \) the bottom surface of the build plate where the fixed support is imposed; on the remaining part of the boundary \( \partial \Omega \), we impose homogeneous Neumann boundary conditions.

2.2. Numerical approach

In the present work, we use Ansys2021-R2 software to simulate the beam PBF-LB/M process, which adopts a weakly coupled thermomechanical approach based on the FE method [37]. This means that the thermal and mechanical analyses are not fully coupled, i.e., they are not solved monolithically at each time step, but rather in a staggered way, allowing the calculations to be greatly speeded up. In particular, the thermal transient analysis is solved first throughout the printing time by storing the thermal field at each layer. These temperature fields are then transferred to the quasi-static mechanical problem solver, where they are used to evaluate the thermal strain of the problem (see Equation (11)).

2.2.1. Meshing strategy

We adopt two different meshing strategies for the component and the build plate. In particular, for the discretization of the component, we use a uniform mesh with quadratic hexahedral finite elements of size 0.5 mm; while for the build plate we choose a coarser mesh, with linear hexahedral finite elements of size 3 mm. This choice is motivated by the fact that the build plate is modeled only to take into account the heat loss through the build plate and as a mechanical constraint for the component, so it does not require accurate meshing. Since the two meshes are non-conforming at the interface, their coupling is achieved by a contact element approach (see [38]).

2.2.2. Material Properties

The material for the build plate and the component is set to be the nickel-based super-alloy Inconel 625. During the PBF-LB/M process – due to the strong thermal gradients – the material reaches temperatures ranging from chamber temperature to temperatures above the melting point. Therefore, we adopt a bilinear isotropic plastic hardening model with a temperature-dependent yield behavior (Figure 2(a)). In Figures 2(b) to 2(f), we report the temperature-dependent material properties used in the present work, whereas the temperature-independent material density and the melting temperature are set to 8440 kg/m³ and 1290 °C, respectively.

2.2.3. Printing parameters

To simulate the melting and solidification process during the construction of a single layer, we assume a total layer process duration of 52 s in which, in the first 26 s, the entire layer is heated and, in the following 26 s, it is cooled down to a temperature of 20 °C. Due to the part-scale nature of our model, at each new layer activation, we do not model the localized laser heat source but, instead, we set the entire newly activated layer at a so-called activation temperature, \( T_A \).

The material deposition process is modeled via the element birth and death technique [7]. In such a technique, the FE models of both the component and the build plate are initially completely constructed, then all elements contained in the component model are deactivated. Deactivated elements remain in the FE model but contribute with only a very small conductivity value to the total system, i.e., their contribution to the problem is negligible. Only once a new powder layer is activated, all deactivated elements within that layer are switched to active elements, i.e., the actual material conductivity value is assigned to the element. More details can be found in [7, 37].

To simulate the printing environment, we set the temperature of the top surface of the build plate to 80 °C while the side surfaces are set to 40 °C to contain thermal gradients. At the end of the printing process, we assume that the build plate is cooled down to the chamber temperature set at 20 °C. Finally, we also assume that at the end of the printing process the component is partially removed from the build plate as depicted in Figure 1.
Figure 2: Temperature-dependent Inconel 625 properties.
the activation temperature $T_A$ see Table 1. Note that, while we could have considered $h$ assume that each parameter is a uniform random variable over a suitable range, and that these three random variables as random variables. Moreover, since we want to enforce as little prior knowledge as possible on the parameters, we consider as uncertain in our study are the logarithm (in base 10) of the powder convection coefficient, log $h_p$ (see Section 2.1.1), the logarithm of the gas convection coefficient, log $h_g$ (see Section 2.1.1), and the activation temperature $T_A$ (see Section 2.2.3). As usual in UQ, these uncertain parameters are initially modeled as random variables. Moreover, since we want to enforce as little prior knowledge as possible on the parameters, we assume that each parameter is a uniform random variable over a suitable range, and that these three random variables are mutually independent; for the same reason, we take intervals larger than those typically used in literature [39–44], see Table 1. Note that, while we could have considered $h_p$ and $h_g$ as random variables themselves rather than their logarithm, this latter choice is more effective since it allows us to easily span a large range of values, giving at the same time equal importance in the numerical investigation to both the smaller end and the larger end of the interval where $h_p$ and $h_g$ live (specifically $[10^{-5}, 10^0]$); in other words, with this choice small values of $h_p$, $h_g$ (say in the range from $10^{-5}$ to $10^1$) are investigated as thoroughly as the larger values.

The objective of the inverse UQ analysis that we will perform in this work is to compute a new PDF in which some values of the parameters are “more probable” than others, because they match better with the available data. In other words, we aim at incorporating the information from the data at disposal in the modeling of the uncertainty of the three parameters considered. We collect the three uncertain parameters in a vector $v = (v_1, v_2, v_3) = (T_A, \log h_g, \log h_p)$ and introduce some notation that will be used in the following:

- $\Gamma_n = [a_n, b_n]$ is the range of each uncertain parameter $v_n$ with $n = 1, 2, 3$;
- $\Gamma = \Gamma_1 \times \Gamma_2 \times \Gamma_3$ is the domain of $v$, i.e., the hyper-rectangle $[a_1, b_1] \times [a_2, b_2] \times [a_3, b_3]$;
- $\rho_n(v_n)$ is the PDF of $v_n$. Given the discussion above, we have $\rho_{n, \text{prior}}(v_n) = \frac{1}{b_n - a_n}$, where the subscript “prior” denotes the fact that such PDF incorporates only the prior information in Table 1. After the inverse UQ procedure, these PDFs will be updated to a data-informed posterior PDF, indicated as $\rho_{n, \text{post}}$;
- $\rho(v)$ is the joint PDF of the vector $v$. In particular, $\rho_{\text{prior}}(v)$ and $\rho_{\text{post}}(v)$ are the joint prior and posterior PDFs of $v$, respectively. Given the assumption that the three parameters are a-priori mutually independent, we have $\rho_{\text{prior}}(v) = \prod_{n=1}^{3} \rho_{n, \text{prior}}(v_n)$; instead, we cannot assume at this stage that $\rho_{\text{post}}$ factorizes as $\rho_{\text{post}} = \prod_{n=1}^{3} \rho_{n, \text{post}}(v_n)$, since we do not have (yet) information on the statistical independence of $v_n$ after the inversion;
- we will write $w(x, v)$ to denote the displacement along the $z$-direction at $x \in \Omega$ corresponding to the value $v$ of the parameters;
- more generally, $f(v) : \Gamma \rightarrow \mathbb{R}^P$ denotes any QoI (output) of the simulation (displacements, residual strains) and emphasizes that such quantities are function of $v$. When $P = 1$ (scalar-valued QoI), we use the notation $f(v)$.

### Table 1: Parameter spaces of the PBF-LB/M process simulation chosen for the inverse UQ analysis.

| random variables | units | range $[a_n, b_n]$ |
|------------------|-------|--------------------|
| Activation temperature ($T_A$) | °C | [1130; 1450] |
| log of gas convection coefficient ($\log h_g$) | | $[-5, 0]$ |
| log of powder convection coefficient ($\log h_p$) | | $[-5, 0]$ |

3. Uncertainty Quantification

#### 3.1. Sources of uncertainty

The parameters that we consider as uncertain in our study are the logarithm (in base 10) of the powder convection coefficient, log $h_p$ (see Section 2.1.1), the logarithm of the gas convection coefficient, log $h_g$ (see Section 2.1.1), and the activation temperature $T_A$ (see Section 2.2.3). As usual in UQ, these uncertain parameters are initially modeled as random variables. Moreover, since we want to enforce as little prior knowledge as possible on the parameters, we assume that each parameter is a uniform random variable over a suitable range, and that these three random variables are mutually independent; for the same reason, we take intervals larger than those typically used in literature [39–44], see Table 1. Note that, while we could have considered $h_p$ and $h_g$ as random variables themselves rather than their logarithm, this latter choice is more effective since it allows us to easily span a large range of values, giving at the same time equal importance in the numerical investigation to both the smaller end and the larger end of the interval where $h_p$ and $h_g$ live (specifically $[10^{-5}, 10^0]$); in other words, with this choice small values of $h_p$, $h_g$ (say in the range from $10^{-5}$ to $10^1$) are investigated as thoroughly as the larger values.

The objective of the inverse UQ analysis that we will perform in this work is to compute a new PDF in which some values of the parameters are “more probable” than others, because they match better with the available data. In other words, we aim at incorporating the information from the data at disposal in the modeling of the uncertainty of the three parameters considered. We collect the three uncertain parameters in a vector $v = (v_1, v_2, v_3) = (T_A, \log h_g, \log h_p)$ and introduce some notation that will be used in the following:

- $\Gamma_n = [a_n, b_n]$ is the range of each uncertain parameter $v_n$ with $n = 1, 2, 3$;
- $\Gamma = \Gamma_1 \times \Gamma_2 \times \Gamma_3$ is the domain of $v$, i.e., the hyper-rectangle $[a_1, b_1] \times [a_2, b_2] \times [a_3, b_3]$;
- $\rho_n(v_n)$ is the PDF of $v_n$. Given the discussion above, we have $\rho_{n, \text{prior}}(v_n) = \frac{1}{b_n - a_n}$, where the subscript “prior” denotes the fact that such PDF incorporates only the prior information in Table 1. After the inverse UQ procedure, these PDFs will be updated to a data-informed posterior PDF, indicated as $\rho_{n, \text{post}}$;
- $\rho(v)$ is the joint PDF of the vector $v$. In particular, $\rho_{\text{prior}}(v)$ and $\rho_{\text{post}}(v)$ are the joint prior and posterior PDFs of $v$, respectively. Given the assumption that the three parameters are a-priori mutually independent, we have $\rho_{\text{prior}}(v) = \prod_{n=1}^{3} \rho_{n, \text{prior}}(v_n)$; instead, we cannot assume at this stage that $\rho_{\text{post}}$ factorizes as $\rho_{\text{post}} = \prod_{n=1}^{3} \rho_{n, \text{post}}(v_n)$, since we do not have (yet) information on the statistical independence of $v_n$ after the inversion;
- we will write $w(x, v)$ to denote the displacement along the $z$-direction at $x \in \Omega$ corresponding to the value $v$ of the parameters;
- more generally, $f(v) : \Gamma \rightarrow \mathbb{R}^P$ denotes any QoI (output) of the simulation (displacements, residual strains) and emphasizes that such quantities are function of $v$. When $P = 1$ (scalar-valued QoI), we use the notation $f(v)$.

#### 3.2. Uncertainty Quantification workplan

The fundamental premise of UQ is the observation that since $v$ is uncertain and described by a random vector with an associated PDF, any output $f(v)$ is also an uncertain quantity. Computing efficiently the PDF of $f(v)$ is the final goal of the UQ analysis; in particular, the QoI that we will ultimately consider in this work are the residual strains along the beam. To this end, we will proceed accordingly to the workplan detailed below, whose steps will be described in

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In the following subsections; note in particular that we will assume of having at disposal data (measurements) about another QoI of the model, namely, the displacements of the beam. Accordingly, the workplan is as follows.

1. Global Sensitivity Analysis (GSA for short, see Section 3.4): we investigate how much each uncertain parameter \( v_n \) contributes to the variability of the displacements. The finding of this analysis is that the second parameter, i.e., the gas convection coefficient, has little impact on the displacements and therefore can be fixed to a constant value in the subsequent analyses. This reduces the dimensionality of the problem and therefore the computational costs of the next two steps. In particular, the new PDF to be considered is now \( \rho_{\text{prior,red}}(v) = \rho_1(v_1)\rho_3(v_3) \) and the reduced parameter space is \( \Gamma_{\text{red}} = \Gamma_1 \times \Gamma_3 \).

2. Inverse UQ (see Section 3.5): by relying on Bayesian inversion techniques, we update the initial PDF \( \rho_{\text{prior,red}} \) of the two remaining uncertain parameters, incorporating the information coming from available data on displacements. The result is a new PDF, \( \rho_{\text{post}} \), tailored to the data at hand. Such new PDF has a “reduced uncertainty”, i.e., a smaller variance, compared to \( \rho_{\text{prior,red}} \).

3. Posterior-based forward UQ (see Section 3.6): we sample \( \Gamma_{\text{red}} \) according to the PDF \( \rho_{\text{post}} \) just derived and evaluate the corresponding residual strains. From these values, we finally compute the PDF of the residual strains.

### 3.3. Speeding up uncertainty quantification by sparse-grid surrogate modeling

All the steps in the workplan above require repeatedly solving the PBF-LB/M model for different values of \( v \) to evaluate the corresponding QoIs \( f(v) \) (displacements, residual strains). Specifically, in GSA we need to assess how much changing the value of each \( v_n \) impacts the value of the displacements. In the inverse UQ we instead need to test the compatibility of each value of \( v \) with the available displacement data: intuitively, if for certain values of \( v \) the solution of the model is “far” from the data, such values of the parameters are “unlikely”, and therefore the corresponding values of \( \rho_{\text{post}}(v) \) must be small. Finally, in forward UQ we need to obtain values of the strains to compute their PDF.

To reduce the computational burden, in the following we replace the values of \( f(v) \) resulting from the evaluation of the PBF-LB/M model with suitable approximations, obtained building so-called surrogate models of \( f(v) \). Surrogate models are typically obtained with a two-step procedure. In the first step (“offline step”/ “training step”), we evaluate the PBF-LB/M model for a handful of judiciously chosen values of \( v \), say \( f(v_1), \ldots, f(v_M) \), and then create an approximation of \( f(v) \) out of these \( M \) values, based, e.g., on interpolation, least squares regression, neural networks, etc. In the second step (“online step”/ “evaluation step”), whenever a new value of \( f(v) \) is needed, we evaluate the cheap surrogate model instead of the expensive PBF-LB/M model, with considerable computational savings.

In particular, in this work we consider the so-called sparse-grid surrogate models, that are among the most popular surrogate modeling technique in UQ, see [29–31]. For an overview of alternative methods, we refer to [18]. In this section we explain the basics of sparse grids; more details are provided in Appendix A.

Before giving the definition of sparse-grid surrogate models, we point out that the sparse-grid approximation of a QoI \( f(v) \) depends (among other things) on the number of uncertain parameters, \( N \), and on their PDF; therefore, we will actually need three different sparse-grids surrogate models: the first one for the GSA (3 parameters, \( \rho_{\text{prior}} \)); the second one for the inverse UQ analysis (2 parameters with the restricted \( \rho_{\text{prior,red}} \), the third one for the forward UQ analysis (2 parameters with \( \rho_{\text{post}} \)). Table 2 summarizes the properties used for the three models; the meaning of the different entries will become clearer as we progress with the explanation.

| sparse grid | used in | \( N \) | PDF | \( I \) | \( w \) | univariate nodes | points | surrogate for |
|------------|---------|--------|-----|------|------|----------------|-------|---------------|
| 1          | GSA     | 3      | \( \rho_{\text{prior}} \) | \( I_{\text{max}} \) | 1 | symm. Leja | 27 | 11 \( z \)-displacements |
| 2          | inverse UQ | 2 | \( \rho_{\text{prior,red}} \) | \( I_{\text{sum}} \) | 3 | symm. Leja | 25 | 9 \( z \)-displacements |
| 3          | forward UQ | 2 | \( \rho_{\text{post}} \) | \( I_{\text{sum}} \) | 3 | symm. Leja (log \( h_{p} \)) | 25 | 120 \( x \)-residual strains |

symm. Gaussian Leja (\( T_A \))
we denote by $S_f f(v)$ reads:

$$f(v) = S_f f(v) = \sum_{i \in I} c_i U_i(v), \quad c_i := \sum_{j \in [0,1]^N \atop i+j \in I} (-1)^{|j|},$$

where:

- $i = [i_1, i_2, \ldots, i_N] \in \mathbb{N}_+^N$ is a multi-index, i.e., a vector of $N$ integer positive numbers, $i_n \geq 1$;
- $I$ is a collection of multi-indices, called multi-index set, $I \subset \mathbb{N}_+^N$. It must satisfy a so-called downward-closedness condition, see Appendix A;
- $U_i(v)$ is a tensor Lagrangian interpolant of $f(v)$, built over a Cartesian grid on $\Gamma$ with

$$(2i_1 - 1) \times (2i_2 - 1) \times \cdots \times (2i_N - 1)$$

points. In other words, the $n$-th component of $i$ specifies how many values should be used for $v_n$ when constructing the Cartesian grid on $\Gamma$;
- $c_i$ are the so-called combination technique coefficients. Note that some $c_i$ might be null, in which case $U_i(v)$ is not part of the final approximation.

The sparse-grid surrogate model of $f(v)$ thus consists of a linear combination of several tensor Lagrangian interpolants of $f(v)$, each built over a different Cartesian grid covering the parameter space $\Gamma$. The specific tensor Lagrangian interpolants that form this approximation are dictated by a set $I$; the choice of $I$ is therefore pivotal for the construction of a good sparse-grid surrogate model. The easiest choice of $I$ is certainly

$$I_{\max} = \{ i \in \mathbb{N}_+^N : \max_{n=1\ldots N} (i_n - 1) \leq w \},$$

for some integer $w$. In this case, letting $i_w = [w+1, w+1, \ldots]$, it can be shown that $S_f f(v) = U_i(v)$, i.e., the sparse grid reduces to a tensor Lagrangian interpolant based on $(2w - 1)^N$ points (all $c_i$ are zero other than $c_i_w = 1$). This choice is however unfeasible even for moderate values of $w$ or $N$, since it would require too many evaluations of $f(v)$. A classic (and more reasonable) choice is choosing the set

$$I_{\text{sum}} = \{ i \in \mathbb{N}_+^N : \sum_{n=1\ldots N} (i_n - 1) \leq w \},$$

again for some integer $w$. In this case, the Lagrange interpolants $U_i(v)$ would require to sample extensively only some of the parameters (since $i_w$ would be such that if one component is large, the other ones are small); however, combining them by the coefficients $c_i$, we recover a good approximation of $f(v)$, using significantly less samples than the previous $(2w - 1)^N$. Using the set $I_{\text{sum}}$ ultimately results in a sampling of the parameter space which is structured but not Cartesian; examples can be seen in Section 4.2.1 and Section 4.3.1. In the following we will use the set $I_{\max}$ for the GSA, and $I_{\text{sum}}$ for the inverse and forward UQ analysis.

The set of all points where an evaluation of $f(v)$ is required to build the sparse-grid surrogate model (i.e., the union of all the Cartesian grids of the $U_i(v)$ with $c_i \neq 0$) is actually called sparse grid. Figure 3 shows an example of sparse grid over the space $\Gamma_{\text{red}}$; in particular, the final sparse grid is reported in Figure 3(h), while Figures 3(a) to 3(g) show the breakdown of the sparse grid in Figure 3(h) into the tensor grids composing it.

The final step is to specify how to choose the univariate collocation points over the ranges $\Gamma_n$, i.e., the values of $v_n$ to be used to generate the Cartesian grids over which $U_i(v)$ are built (note that the multi-index $i$ specifies how many points are required for each $v_n$ but not their location). Since $U_i(v)$ are Lagrangian interpolants, using equispaced points is not a good idea, due to the well-known Runge phenomenon [45]; moreover, the points for each $v_n$ should be chosen according to the corresponding PDF for efficiency reason (it is recommended to put more points in regions of high probability). In view of this, we use different families of collocation points for each of the three sparse grids that
we use in this work, see Table 2. Specifically, the sparse grids for the GSA and for the inverse UQ need to be built according to the fact that \( \rho_{\text{prior}} \) and \( \rho_{\text{posterior}} \) consist of uniform PDF, for which we elect to use the so-called symmetric Leja points (see Appendix B for details on their definitions). Instead, for the final forward UQ based on \( \rho \) according to the fact that we use in this work, see Table 2. Specifically, the sparse grids for the GSA and for the inverse UQ need to be built to each component of \( f \) construction to vector-valued quantities of interest. As detailed in Appendix B, both these variants of Leja points are non-equispaced points, obtained minimizing the corresponding Lebesgue constant, and thus are good for interpolation and hence surrogate modeling. Figure 4 shows a set of 9 symmetric Leja points (Figure 4(a)) and 9 symmetric Gaussian Leja points (Figure 4(b)).

Finally, we conclude this overview of sparse grids pointing out that extending the sparse-grid surrogate model construction to vector-valued quantities of interest \( f(v) \) is straightforward. In fact, we need to apply the same procedure to each component of \( f(v) \). In particular, this means that the same set of collocation points (i.e., the same sparse grid) can be used to compute the sparse-grid surrogate model of a vector-valued \( f \).

Now that we have presented the framework of the UQ workflow and the basics of sparse grids, we are ready to explain how each of the three steps of the workplan is performed.
3.4. Global Sensitivity Analysis (GSA)

In the present work, we use the Sobol decomposition method [46–48] to assess the influence of the three uncertain parameters on the displacements. The method is similar to the classical ANOVA decomposition of the variance and consists of computing two sets of indicators, namely the principal and total Sobol indices. The first ones measure the individual contribution of each parameter to the variance of the QoI, while the second ones quantify the contributions of each parameter combined with the others.

As already mentioned, the first step to perform the GSA for the displacements is to build a sparse-grids surrogate model for them. We use the specifics listed in the first row of Table 2, which result in a Cartesian sampling of \( \Gamma \) with \( 3 \times 3 \times 3 = 27 \) symmetric Leja point, meaning that we need to run 27 PBF-LB/M full model simulations. Note that 3 symmetric Leja points over an interval \( \Gamma_n = [a_n, b_n] \) means in practice considering the following three values for the parameter \( v_n \): \( v_n = a_n, b_n, (a_n + b_n)/2 \) (see Appendix B). Once having the sparse grid at hand, deriving the Sobol indices is a relatively easy but quite technical operation, see [49] for details.

The results discussed in Section 4.1 show that the principal and total Sobol indices for \( \log h_p \) are small compared to the others and thus \( \log h_p \) can be neglected in the following steps of the UQ workflow; in practice, this means that from now on, \( \log h_p \) can be fixed to a convenient value. As a consequence for the inverse and forward UQ analysis we consider a reduced parameter space \( \Gamma_{\text{red}} = \Gamma_1 \times \Gamma_3 \) and the new PDF \( \rho_{\text{prior,red}}(v) = \rho_1(v_1)\rho_3(v_3) \). Note that with a slight abuse of notation, in the following, \( v \) denotes also the reduced vector \( v = (T_A, \log h_p) \); the context will always make clear whether \( v \) denotes the reduced \( v = (T_A, \log h_p) \) or the original \( v = (T_A, \log h_e, \log h_p) \).

3.5. Inverse UQ analysis

In the present work, we adopt a Bayesian inversion approach [20–22] to perform the inverse UQ analysis. More specifically, Bayesian inversion consists in updating the PDF of the two remaining uncertain parameters \( T_A, \log h_p \) from the uniform \( \rho_{\text{prior,red}} \) to a new posterior PDF \( \rho_{\text{post}} \), that incorporates the fact that we have at disposal a set of measurements of displacements of the beam at \( K \) positions \( x_{k,\text{meas}}, \ldots, x_{K,\text{meas}} \) (see Section 4.2.1 for details on the locations of \( x_{k,\text{meas}} \)).

Ideally, we would like to use actual experimental measures of displacements in the inverse UQ analysis. However, as a preliminary step towards future work, in the present manuscript we consider instead a set of imperfect (noisy) synthetic data \( \tilde{u} \) obtained by first running the part-scale thermomechanical model for a set of parameters of our choice denoted with \( \Psi \) (target values), and then adding to such displacement field a set of \( K \) independent Gaussian noises to mimic measurement error, as follows:

\[
\begin{align*}
\tilde{u}_k &= u(x_{k,\text{meas}}, \Psi) + \epsilon_k, & k = 1, \ldots, K \\
\epsilon_k &\sim N(0, \sigma^2_{\epsilon_k}).
\end{align*}
\]

This allows us to focus on the methodological aspect of the inversion, removing from the analysis any error due to the inadequacy of the computational model to represent reality. Furthermore, for simplicity, in the following \( \sigma_{\epsilon_k} \) is assumed to be constant, i.e., \( \sigma_{\epsilon_k} = \sigma \forall k \).

To begin with the Bayesian inversion, we introduce the misfits \( M_k(\Psi) \) between the synthetic data and the displacements predicted by the model when the parameters have value \( \Psi \), i.e.:

\[
M_k(\Psi) := \tilde{u}_k - u(x_{k,\text{meas}}, \Psi), \quad k = 1, \ldots, K.
\]

The posterior PDF \( \rho_{\text{post}} \) is calculated using Bayes’ theorem [20, 21] as follows:

\[
\rho_{\text{post}}(v) = \mathcal{L}(v | \tilde{u}_k) \rho_{\text{prior}}(v) \frac{1}{C},
\]

where \( C \) is a normalization constant that makes \( \rho_{\text{post}}(v) \) actually a PDF (i.e., its integral equal to 1) and \( \mathcal{L}(v | \tilde{u}_k) \) is the so-called likelihood function, which quantifies the plausibility (“likelihood”) of \( v \) given the displacement data, i.e., the plausibility that the measured displacements were generated by \( v \) rather than by the actual \( \tilde{v} \) (that in the general scenario would be unknown). As we are assuming independent Gaussian distributions for the measurement noises,
see Equation (15), the likelihood \( L(v | \tilde{u}_k) \) is

\[
L(v | \tilde{u}_k) = \prod_{k=1}^{K} \frac{1}{\sqrt{2\pi \sigma_k^2}} e^{-\frac{(v_k - \tilde{u}_k)^2}{2\sigma_k^2}},
\]

i.e., the joint probability of observing the misfits \( M_1, \ldots, M_K \) corresponding to the value \( v \) of the parameters.

We now recall that the final goal of the UQ analysis (step 3 of the UQ workflow) is to sample extensively \( \rho_{\text{post}} \) according to \( \rho_{\text{post}} \), to obtain the PDF of the residual strains given the data (posterior-based forward UQ). Sampling \( \rho_{\text{post}} \) as in Equation (17) can be done by means of Markov-Chain Monte Carlo (MCMC) methods [50], which can be however quite computational intensive. A significant reduction in computational costs can be obtained upon assuming that \( \rho_{\text{post}} \) is well-approximated by a Gaussian PDF [22], with appropriate mean vector and covariance matrix (we will discuss the validity of this assumption later), which is standard to sample from. We therefore devote the next subsection to detailing how to compute the mean and covariance matrix of the Gaussian approximation of \( \rho_{\text{post}} \): this is where the second sparse grid in Table 2 comes in handy.

3.5.1. Gaussian approximation of \( \rho_{\text{post}} \)

The mean of the Gaussian approximation can be taken as the maximum of the posterior PDF, \( v_{\text{MAP}} \) (Maximum A Posteriori), as follows:

\[
v_{\text{MAP}} := \arg \max_{v_{\text{grid}}} \rho_{\text{post}} = \arg \max_{v_{\text{grid}}} L(v | \tilde{u}_k),
\]

where the second equality is due to the fact that \( \rho_{\text{prior}} \) and \( C \) are constants. It is easy to see that this maximization is in practice equivalent to the classical least squares approach for the calibration of \( v \), i.e., the minimization of the sum of squared errors \( LS \):

\[
v_{\text{MAP}} = \arg \min_{v_{\text{grid}}} \sum_{k=1}^{K} M_k^2(v),
\]

\[
LS(v) = \sum_{k=1}^{K} M_k^2(v).
\]

The functional \( - \log L(v | \tilde{u}_k) \) appearing in the first equality of Equation (20) is known in the Bayesian literature as negative log-likelihood functional. Note that the minimization in Equation (20) requires evaluating multiple times the functional \( LS(v) \), and thus running multiple times the PBF-LB/M model to obtain the displacements \( u(x_{k,\text{meas}}, v) \) for different values of \( v \). To reduce this cost, we replace \( u(x_{k,\text{meas}}, v) \) by the sparse-grids surrogate model detailed in the second row of Table 2, i.e., we modify the definition of the misfits as

\[
M_k(v) := \tilde{u}_k - S_{\text{red}}(x_{k,\text{meas}}, v), \quad k = 1, \ldots, K.
\]

As reported in Table 2, we need 25 PBF-LB/M evaluations to build this new surrogate model, which is much less than the number of evaluations of the model requested by the optimization procedure. Of course, replacing the exact \( u(x_{k,\text{meas}}, v) \) with its sparse-grid surrogate \( S_{\text{red}}(x_{k,\text{meas}}, v) \) introduces an error, which needs to be small enough: in Section 4.2.1 we present a numerical procedure to check that this is actually the case (surrogate model validation).

Once \( v_{\text{MAP}} \) has been computed, the final step is to derive the covariance matrix of the Gaussian approximation of \( \rho_{\text{post}} \). Such a matrix can be computed as:

\[
\Sigma_{\text{post}} = \tilde{\sigma}_{\text{MAP}}^2 \left( J_u^T J_u + \sum_{k=1}^{K} M_k H_{\tilde{u}_k} \right)^{-1},
\]

where:

* \( \tilde{\sigma}_{\text{MAP}}^2 \) is an approximation of \( \sigma^2 \) (typically unknown for actual experimental data), that we can obtain using the
standard sample variance estimator:

\[ \hat{\sigma}^2 \approx \hat{\sigma}_{MAP}^2 = \frac{1}{K} \sum_{k=1}^{K} (\tilde{u}_k - u(x_{k,\text{meas}}, \mathbf{v}_{\text{MAP}}))^2 = \frac{1}{K} LS(\mathbf{v}_{\text{MAP}}); \]  

- \( J_u \) is the Jacobian matrix with respect to \( \mathbf{v} \) of the displacements at the measuring location evaluated at \( \mathbf{v}_{\text{MAP}} \), i.e., the following \( K \times 2 \) matrix:

\[
J_u = \begin{bmatrix}
\nabla^T_{x} u(x_{1,\text{meas}}, \mathbf{v}_{\text{MAP}}) \\
\nabla^T_{x} u(x_{2,\text{meas}}, \mathbf{v}_{\text{MAP}}) \\
\vdots \\
\nabla^T_{x} u(x_{K,\text{meas}}, \mathbf{v}_{\text{MAP}}) 
\end{bmatrix};
\]

- \( H_{\mathbf{h}} \) is the Hessian of \( u(x_{k,\text{meas}}, \mathbf{v}) \) with respect to \( \mathbf{v} \), evaluated at \( \mathbf{v}_{\text{MAP}} \) (i.e., a \( 2 \times 2 \) matrix).

Also for these computations, it is helpful to use the sparse-grid surrogate model for \( u(x_{k,\text{meas}}, \mathbf{v}) \), thanks to which we can cheaply compute finite difference approximations of the first and second partial derivatives of \( u(x_{k,\text{meas}}, \mathbf{v}) \) with respect to \( \mathbf{v} \).

3.5.2. A mixed Gaussian-uniform approximation of \( p_{\text{post}} \)

As we have already mentioned, the validity of the Gaussian approximation of \( p_{\text{post}} \) must be checked. Since in this work we consider only two parameters in the inverse UQ procedure (\( T_A \) and log \( h_p \)), this check can be easily done by plotting the isolines of the posterior PDF (or equivalently of the negative log-likelihood functional or of the least squares functional), and verifying that such isolines are shaped as ellipses in the proximity of \( \mathbf{v}_{\text{MAP}} \). In our case, this is unfortunately not true: in Figure 10, we can see that the isolines form a band/strip surrounding \( \mathbf{v}_{\text{MAP}} \). This suggests that a Gaussian approximation of \( p_{\text{post}} \) is not appropriate; more numerical evidence about this fact is discussed in Section 4.2.2. The shape of the isolines actually suggests a mixed approach, in which the posterior PDF of \( T_A \) is taken as Gaussian and the posterior PDF for log \( h_p \) as uniform on a smaller interval than the prior one. Furthermore, the fact that the isolines are parallel to the axis of log \( h_p \) suggests that the two parameters can be still considered as statistically independent, implying that \( p_{\text{post}} \) can be finally taken as the product of the two new PDFs for \( T_A \) and log \( h_p \). More in detail, the mean of the Gaussian PDF for \( T_A \) can be taken as the first entry of \( \mathbf{v}_{\text{MAP}} \) and the variance can still be taken as the element (1, 1) of the covariance matrix \( \Sigma_{\text{post}} \) presented above (that is hopefully smaller than the variance in the prior distribution), while the new interval for log \( h_p \) can be chosen by heuristic considerations that we will present in Section 4.2.2.

3.6. Posterior-based forward UQ analysis

The final goal of the present work is to perform a forward UQ analysis based on the (data-informed) posterior PDF of the parameters, to quantify the uncertainty in the prediction of the residual strains of the beam given the uncertainty on the parameters \( T_A \) and log \( h_p \), now modeled by \( p_{\text{post}} \). More precisely, our aim is to approximate the PDF of the residual strains at \( L \) locations \( x_{j,\text{str}} \) along the x-direction (\( \varepsilon_{xx}(x_{j,\text{str}}, \mathbf{v}) \)) of the beam (see Section 4.3.1 for details on the locations of \( x_{j,\text{str}} \)).

To this end, we first generate a sparse-grid surrogate model for the residual strains \( \mathcal{S}_{T_{1,\text{str}} \varepsilon_{xx}}(x_{j,\text{str}}, \mathbf{v}) \) at each of the \( L \) locations, using the specifics listed in the third row of Table 2. We then check that the accuracy with which such sparse-grid surrogate models approximate the full model residual strains \( \varepsilon_{xx}(x_{j,\text{str}}, \mathbf{v}) \) is enough for our purposes (see Section 4.3). To do this, we generate 10000 samples of \( \mathbf{v} \) according to \( p_{\text{post}} \), and for each of these values we approximate the residual strains \( \varepsilon_{xx}(x_{j,\text{str}}, \mathbf{v}) \) by evaluating the sparse-grid surrogates \( \mathcal{S}_{T_{1,\text{str}} \varepsilon_{xx}}(x_{j,\text{str}}, \mathbf{v}) \). Finally, we approximate the residual strain PDF at each location by applying a kernel density estimate method [51, 52] to the 10000 residual strain values obtained by the surrogate models at each location.

4. Results and discussion

All the simulations of the PBF-LB/M process discussed in this section are obtained on an HPC server equipped with a CPU with 128 AMD EPYC 7702@1.67 GHz cores and 376 GB RAM. The UQ analyses are implemented in Matlab, relying on the Sparse-Grids Matlab-Kit [32].
4.1. Global sensitivity analysis

The GSA analysis on the displacements described in Section 3.4 is performed considering as QoI the displacements at the centers of the eleven ridges of the beam (see Figure 1), i.e., a vector-valued QoI with components $f_j(v) = u(x_{j,GA}, v)$ for $j = 1, \ldots, 11$, returning 11 sets of Sobol indices, as displayed in Figure 5. The sets corresponding to the first 8 ridges further from the end of the removal area (Figure 1) are similar, whereas the remaining 3 sets are unreliable due to their proximity to the end of the removal area and thus we neglect them in the subsequent analyses. The results indicate that the parameters with the greatest principal and total Sobol indices, i.e. with the greatest influence on the displacements, are $T_A$ and $\log h_p$ while $\log h_g$ has a negligible effect. This allows us to continue our study by treating as uncertain only the activation temperature and the powder convection coefficient, setting $\log h_g = -5$ (i.e., $h_g = 10^{-5}$ W/(mm$^2$ °C$^{-1}$)) for subsequent analyses.

4.2. Inverse UQ

4.2.1. Surrogate model for inverse UQ

We then construct a new sparse-grid surrogate model depending on $T_A$ and $\log h_p$ only, to be used within the inverse UQ analysis. As already mentioned, the new sparse grid employs the set $\mathcal{I}_{sum}$ and is based on 25 evaluations of the PBF-LB/M model (cf. row 2 of Table 2), corresponding to the points reported in Figure 6(a). Note that also here we consider a vector-valued QoI, with components $f_k(v) = u(x_{\text{meas}, k}, v)$ for $k = 1, \ldots, 9$, i.e., we consider 9 measurement locations $x_{\text{meas}, k}$, that we set at the first 5 ridges and at the 4 midpoints between the respective ridges up to $x = 28.5$ mm (see Figure 1; the 4 midpoints are those with labels from “a” to “d”). This choice guarantees that the measurement locations are at a sufficient distance from the end of the removal area, set at $x = 56$ mm (Figure 1), whose results could be affected by numerical instabilities. The corresponding 9 surrogate models behave similarly, therefore in the rest of this section we show results about the first node (ridge) of the beam. In Figure 6(b) we report the surrogate model $S_{\text{meas}}(x_{\text{meas}}, v)$, which shows a monotonically increasing behavior with respect to both parameters.

Before proceeding with the inversion, we evaluate the quality of the sparse-grid surrogate model through a convergence test. In detail, we generate $M = 50$ random couples $v = (T_A, \log h_p)$ and for each of them we compute the displacements at the 9 locations; then, we generate the sparse grids corresponding to the specifics in row 2 of Table 2 for increasing $w = 0, 1, 2, 3$. For each of these grids we compute the surrogate model predictions of the displacements at the same locations. Finally, we compute the following pointwise prediction errors, $E_{PPE}$, and the root mean square
Figure 6: Surrogate model construction for the inverse UQ analysis.

(a) Sparse grid

(b) Surrogate model

Figure 7: Results of the sparse-grid surrogate model for inverse UQ analysis convergence test at the first node of the beam.

(a) Pointwise prediction error $E_{PPE}$

(b) Root mean square error $E_{MSE}$

The results of the convergence test reported in Figures 7(a) and 7(b) show that the sparse-grid surrogate model with $w = 3$ (25 sparse-grid points) can be considered suitable for the inverse UQ analysis, since the maximum relative error is approximately 1%, and the root mean square error is even smaller. The effectiveness of the surrogate model can be further appreciated by comparing the displacements obtained from the full model analyses with those obtained from the sparse-grid surrogate model, as shown in Figure 8. In fact, it can be seen that, as the number of sparse-grid points increases (i.e., increasing $w$), the displacements obtained from the surrogate model align with those obtained from the full model analyses to an extent that can be considered sufficiently accurate for our purpose.

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4.2.2. Bayesian inversion

As discussed in Section 3.5, to perform the Bayesian inversion we consider as data the synthetic displacements $\tilde{u}_k$, $k = 1, \ldots, 9$ generated according to Equation (15) setting $\tilde{\sigma} = 10^{-2}$ and target values $\tilde{v} = (T_A; \log h_p) = (1339.8 \, ^\circC; -3.75)$. The measuring locations $x_{k,\text{meas}}$ are the same as in the previous subsection. We consider these data sufficient for our purpose; in fact, additional tests with more data did not change the essence of the results shown below.

We begin by computing the mean of the Gaussian approximation of $\rho_{post}$, i.e., $\mathbf{v}_{\text{MAP}}$ (see Equation (20)). This can be obtained by using, e.g., the gradient-free optimization algorithm Nelder-Mead (available in Matlab through the fminsearch command) to find the minimum of the $LS$ function (Figure 10(a)). To make the result more robust, we repeat the optimization several times, for different initial points of the optimization algorithm. Proceeding in this way, we find three local minimum points, see Figure 10(b), one of which falls outside the chosen activation temperature range (see Table 1) and thus can be discarded. The two remaining minimum points have very similar values of $T_A \approx 1341 \, ^\circC$, but are very different in terms of $\log h_p$, one being approximately −5 and the other approximately −3. This shows that a Gaussian approximation of the posterior PDF of $\log h_p$ is inappropriate. This consideration is further supported by inspection of the isolines of $LS$ in the area of the minima, that do not have the shape of ellipses, but rather form a band/strip, as already hinted in Section 3.5.2. Therefore, we employ the mixed approximation strategy already presented in Section 3.5.2: we approximate the posterior PDF $\rho_{post}(\mathbf{v})$ as the product of a Gaussian PDF for $T_A$ and of a uniform PDF for $\log h_p$. In details:

- the Gaussian PDF for $T_A$ is centered at the common value of the first component of the two minimum points of $LS(\mathbf{v})$, i.e., at $T_A = 1341 \, ^\circC$, while the standard deviation $\sigma_{T_A,post}$ is taken as the square root of the entry (1, 1) of the covariance matrix $\Sigma_{post}$ (see Equation (22)), resulting in $\sigma_{T_A,post} \approx 13 \, ^\circC$, see Figure 11(a);
- as extrema of the uniform PDF for $\log h_p$ we employ $(-5; -1.5)$, since the profile of the likelihood functional or LS (Figure 11(b)) at $T_A = 1341 \, ^\circC$ as a function of $\log h_p$ is substantially larger outside this interval.

The results are summarized in Table 3. Finally, we verify that the approximation $\tilde{\sigma}_{MAP}^2$ of $\tilde{\sigma}^2$ is good (see Equation (23)); in fact, $\tilde{\sigma}^2$ is fixed at 0.01 and the value of $\tilde{\sigma}_{MAP}^2$ is 0.00767.

4.3. Posterior-based forward UQ for residual strains

The final step of the UQ workflow consists in the posterior-based forward UQ analysis. In particular, we focus on the residual strains $\varepsilon_{zz}(x_{j,\text{str}})$ at $L = 120$ positions $x_{j,\text{str}}$ in the central plane of the beam at $z = 11 \, \text{mm}$ (see dotted green line in Figure 1) obtained according to the PDF $\rho_{post}$ just derived (see Table 3).
Figure 9: Displacements \( u(x_{\text{meas}}, \bar{v}) \) obtained from part-scale thermomechanical analysis (red curve) and synthetic displacements data \( \tilde{u} \) (black markers).

Figure 10: Inverse UQ analysis.

(a) Surface plot of the least-squares functional \( LS(v) \)

(b) Isolines of \( LS(v) \), target value set \( \bar{v} \) and the two local minima computed by minimization of \( LS(v) \)

Table 3: PDF of the parameters resulting from the inverse UQ analysis and used as input for the posterior-based forward UQ analysis.

| Random Variables  | posterior PDF            |
|-------------------|--------------------------|
| \( T_A \) [°C]    | Gaussian(1341; 13)       |
| \( \log h_p \) [\text{--}] | Uniform(-5, -1.5) |
4.3.1. Surrogate model for posterior-based forward UQ

Since the parameter PDF has changed (Table 3), we start by computing a new set of 120 sparse-grid surrogate models, following row 3 of Table 2. The sparse grid over which these surrogate models are based consists of 25 new collocation points in $\Gamma_{red}$ and is shown in Figure 12(a). Figure 12(b) shows instead the sparse-grid surrogate model for the strains at $\mathbf{x} = (x, y, z) = (1.5, 2.5, 11) \text{ mm}$; a similar interpolating surface is observed for all other locations.

We also perform a convergence test similar to what done for the sparse-grid surrogate model used for the inverse UQ. We therefore evaluate the strains by the full model for $M = 50$ new random values of $\mathbf{v} = (T_A, \log h_p)$ according to $\rho_{post}$, and compare these residual strains with their approximations obtained by the sparse-grid surrogate models with $w = 0, 1, 2, 3$, obtaining the corresponding values for the pointwise prediction error, $E_{PPE}$ (Equation (24)) and the root mean square error, $E_{MS E}$ (Equation (25)). As expected, the trend of errors $E_{PPE}$ and $E_{MS E}$ as $w$ increases is similar for all 120 positions, so we report the result for $\mathbf{x}_{1, str} = (1.5, 2.5, 11) \text{ mm}$, see Figure 13. As can be seen, the convergence test suggests that the surrogate model with $w = 3$ (25 sparse-grid points) can be considered accurate enough for our purposes. The same conclusion can be obtained by looking at Figure 14, which shows that, as the number of sparse-grid points increases, the residual strains obtained from the surrogate model align with the residual strains obtained from the part-scale thermomechanical analyses.

4.3.2. Forward UQ for the strains

After validating the sparse-grid surrogate model, we proceed with the final goal of the forward UQ, i.e., to compute the data-informed PDF of $\varepsilon_{xx}$, as explained in Section 3.6. To see to what extent the inversion process allows us to reduce the uncertainty in the prediction of $\varepsilon_{xx}$, we also repeat the procedure based on the prior-information only, i.e., we build a surrogate model for $S_{I sum} \varepsilon_{xx}$ according to the prior PDFs, sample $T_A$ and $\log h_p$ from such prior PDF and derive the corresponding PDF of $\varepsilon_{xx}$. The results are shown in Figure 15 for 6 locations out of the 120 considered. In addition, by computing the mode of PDF of $\varepsilon_{xx}$ at each of the $L = 120$ locations, we derive the most probable profile of the $\varepsilon_{xx}$. Figure 16 shows such a profile considering both the forward UQ analysis based on $\rho_{prior}$ and on $\rho_{post}$. In both cases, we also report the profiles of the 95% and 5% quantiles of the prior and the posterior PDF of $\varepsilon_{xx}$. It can be clearly seen in Figures 16(a) and 16(b) that having previously performed an inverse UQ analysis reduces the uncertainties in the prediction of the residual strains. In fact, if the uncertainties of parameters $T_A$ and $\log h_p$ had not been reduced, there would have been a significantly larger uncertainty in the prediction of the residual strains. Finally, in Figure 16(b) we also report the residual strains obtained from the part-scale thermomechanical analyses at the target parameter couple, i.e., the $\mathbf{v} = (T_A; \log h_p) = (1339.8 \degree C; -3.75)$.
Figure 12: Surrogate model construction for posterior-based forward UQ.

Figure 13: Results of the sparse-grid surrogate model convergence test for the first node (ridge) of the beam as the sparse-grid points increases.
Figure 14: Comparison between sparse-grid surrogate model displacements and part-scale thermomechanical model displacements for the first beam node.

Figure 15: Residual strain PDF of the Inconel 625 beam at $z = 11$ mm based on prior and posterior distribution.
5. Conclusions

In the present work, we quantify and reduce the uncertainties involved in the PBF-LB/M process of a part-scale thermomechanical model of an Inconel 625 beam using synthetic data. We first perform a GSA, by calculating the principal Sobol and total Sobol indices, to study the sensitivity of the AM model to the activation temperature and the gas and powder convection coefficients. This analysis allows us to set the gas convection coefficient to an arbitrary but fixed value since the AM model is essentially insensitive to this parameter. Then, applying an inverse UQ approach, we quantify the uncertainties associated to the activation temperature and the powder convection coefficient. In particular, we do not only provide the point estimate of the uncertain parameters, but also estimate the residual uncertainties of such parameters. A posterior-based forward UQ is subsequently performed to predict residual strains and their associated PDFs. We employ different sparse-grid surrogate models to reduce the computational cost of the numerous analyses required by the UQ methodology (the whole procedure, GSA + inverse UQ + forward UQ, only requires 177 part-scale thermomechanical analyses, of which 100 are only used for validation purposes). The results show the ability of the proposed approach to reduce the uncertainties of the powder convection coefficient and the activation temperature. Finally, our results show how the prediction of residual strains based on posterior uncertainties is significantly more accurate than the prediction of residual strains based on prior uncertainties and how surrogate models are effective for our purposes. As further outlook of the present work, we aim at extending the presented results considering more than one discretization of the FE model, i.e., adopting a multi-fidelity UQ approach such as the so-called multi-index stochastic collocation method [53–55], that extends the presented sparse-grid methodology to the case of multiple solvers. Moreover, since the accuracy of the proposed approach has been verified, experimental measurements can be employed as target data, instead of synthetic ones, in forthcoming works.

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Appendix A. Sparse grid surrogate modeling

In the present section we present the sparse grid surrogate modeling approach adopted for our study. Following the notation introduced in Section 3, we consider the problem of approximating an $N$-variate scalar function $f(v): \Gamma \mapsto \mathbb{R}$, where $v \in \Gamma \subset \mathbb{R}^N$ (extension to $F$-valued functions $F: \Gamma \mapsto \mathbb{R}^F$ is immediate; it is enough to apply the same procedure to each component of $F$). We also recall that $v_n$ are independent random variables with probability density function $\rho_n(v_n), n = 1, \ldots, N$ and that therefore the joint probability density of $v$ over $\Gamma$ is the product $\rho(v) = \prod_{n=1}^{N} \rho_n(v_n)$.

The first step in constructing the sparse-grid surrogate model is to define a set of collocation points for each parameter $v_n$. We denote the number of points along $v_n$ by $K_n \in \mathbb{N}_+$, and define a discretization level for each parameter, i.e., a positive number $i_n \in \mathbb{N}_+$, $i_n \geq 1$, using a “level-to-knots” function $m$ that associates to each level a number of points:

$$m: \mathbb{N}_+ \rightarrow \mathbb{N}_+ \text{ such that } m(i_n) = K_n.$$  

(A.1)

In this work, we have considered $m(i_n) = 2i_n - 1$ (i.e., at each level $i_n$ two more points with respect to the previous level are considered; cf. Equation (14)), but other choices are possible. The set of collocation points at level $i_n$ along parameter $v_n$ is denoted by:

$$T_{i_n} = \left\{ v_{n,m(i_n)}, j_n = 1, \ldots, m(i_n) \right\} \text{ for } n = 1, \ldots, N.$$  

(A.2)

The positions of these points over $\Gamma_n$ is usually chosen on the basis of the PDF $\rho_n$ of the random variables $v_n$. As reported in Table 2, in this work we have used symmetric Leja points whenever $v_n$ is a uniform random variable and symmetric Gaussian Leja points whenever $v_n$ is a Gaussian random variable (see Appendix B for details), but other choices are possible, see e.g. [32]. Our choices have the advantage that Leja points are nested, i.e., $T_{i_k} \subset T_{i_l}$ if $i_k < i_l$.

The second step is the definition of tensor grids of $N$ dimensions, derived as the Cartesian product of the previously introduced univariate sets $T_{i_n}$ and of their associated Lagrangian interpolants. In particular, by collecting the discretization levels $i_n$ in a multi-index $i \in \mathbb{N}_+^N$, considering the corresponding tensor grid $T_i = \bigotimes_{n=1}^{N} T_{i_n}$, with number of nodes $M_i = \prod_{n=1}^{N} m(i_n)$ we can write:

$$T_i = \left\{ v_{m(i)}, j \leq m(i) \right\} \text{ with } v_{m(i)} = \left[ v_{j_1, m(i_1)}, \ldots, v_{j_N, m(i_N)} \right] \text{ and } j \in \mathbb{N}_+,$$

where $m(i) = [m(i_1), m(i_2), \ldots, m(i_N)]$ and $j \leq m(i)$ means that $j_n \leq m(i_n)$ for every $n = 1, \ldots, N$. The tensor-interpolant approximation (also called tensor-interpolant surrogate model) of $f(v)$, that we denote by $\mathcal{U}_i(v)$, is then an $N$-variate Lagrangian interpolant collocated at the grid nodes of $T_i$ and can be written as:

$$f(v) \approx \mathcal{U}_i(v) := \sum_{j \leq m(i)} f \left( \left[ v_{j} \right] \right) \mathcal{L}^{(j)}_{m(i)}(v),$$  

(A.3)

where $\left\{ \mathcal{L}^{(j)}_{m(i)}(v) \right\}_{j \leq m(i)}$ are $N$-variate Lagrange polynomials, defined as tensor products of univariate Lagrange polynomials, i.e.:

$$\mathcal{L}^{(j)}_{m(i)}(v) = \prod_{n=1}^{N} \ell_{n,m(i)}^{(j_n)}(v_n) \text{ with } \ell_{n,m(i)}^{(j_n)}(v_n) = \prod_{k=1, k \neq n}^{m(i)} \frac{v_n - v_{n,m(i)}}{v_{n,k,m(i)} - v_{n,m(i)}}.$$  

The accuracy of the approximation $f(v) \approx \mathcal{U}_i(v)$ increases as the number of collocation points in each $v_n$ grows, i.e., for $i_n \gg 1, n = 1, \ldots, N$. At the same time, the cost of constructing $\mathcal{U}_i(v)$ grows exponentially in $N$, since it requires evaluating $f$ at $M_i = \prod_{n=1}^{N} m(i_n)$ points; this implies that even moderate choices of $i_n, n = 1, \ldots, N$ could be unfeasible for $N > 2$ if evaluating $f$ is an expensive operation. To mitigate this problem, the sparse-grid surrogate model consists of an approximation of $f(v)$ formed by a linear combination of several coarse $\mathcal{U}_i(v)$ rather than by a single $\mathcal{U}_i(v)$ with $i_n \gg 1, n = 1, \ldots, N$. 

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For this purpose, as a third step towards sparse-grid surrogate models we introduce the so-called univariate and multivariate detail operators:

\[ \Delta_n[\mathcal{U}_i(v)] = \mathcal{U}_i(v) - \mathcal{U}_{i-e_n}(v) \text{ with } 1 \leq n \leq N; \quad (A.4) \]

\[ \Delta[\mathcal{U}_i(v)] = \bigotimes_{n=1}^{N} \Delta_n[\mathcal{U}_i(v)] = \Delta_1 [\cdots [\Delta_N [\mathcal{U}_i(v)]]], \quad (A.5) \]

where \( \mathcal{U}_i(v) = 0 \) when at least one component of \( i \) is zero and \( e_n \) the \( n \)-th canonical multi-index, i.e., \( (e_n)_k = 1 \) if \( n = k \) and 0 otherwise. Multivariate detail operators can be evaluated as suitable linear combinations of certain approximations of the complete tensor approximations \( \mathcal{U}_i \):

\[ \Delta[\mathcal{U}_i(v)] = \Delta_1 [\cdots [\Delta_N [\mathcal{U}_i]]] = \sum_{j=0,1}^N (-1)^{|i|} \mathcal{U}_{i-j}(v). \quad (A.6) \]

Moreover, note that a hierarchical decomposition of \( \mathcal{U}_i(v) \) holds:

\[ \mathcal{U}_i(v) = \sum_{j \in I} \Delta[\mathcal{U}_j(v)]. \quad (A.7) \]

The fourth and final step to construct a sparse-grid surrogate model is to tweak such hierarchical decomposition. In detail, instead of summing over \( j \leq i \) we sum over a different collection of multi-indices \( I \) (from here on, multi-index set), chosen according to criteria that will be made clearer in a moment:

\[ f(v) \approx S_I f(v) = \sum_{j \in I} \Delta[\mathcal{U}_j(v)]. \]

Furthermore, applying Equation (A.6) we obtain a more practical expression, i.e., the so-called “combination technique” [56], which is the form actually implemented in the Sparse-Grids Matlab-Kit:

\[ f(v) \approx S_I f(v) = \sum_{j \in I} c_j \mathcal{U}_j(v), \quad c_j := \sum_{j=0,1}^N (-1)^{|j|}. \quad (A.8) \]

This re-writing is valid only if \( I \) is downward-closed, i.e., if \( I \) is such that if a certain multi-index \( i \) is in \( I \) all its “previous” multi-indices \( j \leq i \) are also in the set. In formulae, we require that:

\[ \forall i \in I, \; i - e_n \in I, \quad \forall n = 1, \ldots, N \text{ s.t. } i_n > 0. \quad (A.9) \]

Coming back to the issue of choosing the multi-index set \( I \), the idea is to discard from the hierarchical decomposition in Equation (A.7) the contributions that have a large cost and contribute little to the approximation (in a sense, dropping the high-order corrections). Under mild regularity assumptions of \( f(v) \), a simple yet effective choice to this end is

\[ I_{\text{sum}} = \{ i \in N^+_1^N : \sum_{n=1}^{N} (i_n - 1) \leq w \}; \quad (A.10) \]

for some integer value \( w \) (the larger \( w \), the more accurate is the sparse-grid surrogate model). Note that conversely, choosing

\[ I_{\max} = \{ i \in N^+_1^N : \max_{n=1,...,N} (i_n - 1) \leq w \} \quad (A.11) \]

one would obtain a tensor grid with \( m(w+1) \) points per direction, i.e., \( S_{I_{\text{max}}} f(v) = \mathcal{U}_{i_w}(v) \) with \( i_w = [w+1, w+1, \cdots] \). This is an immediate consequence of the decomposition in (Equation (A.7)). More advanced options to tailor the set \( I \) to the function \( f \) are available in literature, and in particular it would be possible to use an adaptive algorithm, that adds multi-indices \( i \) to \( I \) one by one given the values of \( f \); see again [32] for details. Finally, we call sparse grid the
collection of points needed to build the *sparse-grid surrogate model* $S_T$, i.e.

$$
\mathcal{G}_T = \bigcup_{i \in I_T} \mathcal{G}_i .
$$

**(A.12)**

**Appendix B. Leja points**

Leja knots have been introduced for unweighted interpolation on intervals $[a, b]$, see [32, 57] and references therein, and are therefore a suitable choice when $v_n$ are uniform random variables. They are built recursively as:

$$
\begin{align*}
\nu_n^{(1)} &= b , \quad \nu_n^{(2)} = a , \quad \nu_n^{(3)} = \frac{a + b}{2} , \\
\nu_n^{(j)} &= \arg\max_{v_n \in [a, b]} \prod_{k=1}^{j-1} |v_n - \nu_n^{(k)}| ,
\end{align*}
$$

**(B.1)**

Observe that by construction Leja knots are nested but not symmetric with respect to the mid-point $\frac{a + b}{2}$, which is also a desirable property. To fix this issue, the construction above can be changed by generating only the even elements of the sequence with the standard formula in (Equation (B.1)) and then symmetrizing them to obtain the odd elements, i.e.

$$
\begin{align*}
\nu_n^{(1)} &= b , \quad \nu_n^{(2)} = a , \quad \nu_n^{(3)} = \frac{a + b}{2} , \\
\nu_n^{(2j)} &= \arg\max_{v_n \in [a, b]} \prod_{k=1}^{2j-1} |v_n - \nu_n^{(k)}| , \\
\nu_n^{(2j+1)} &= \frac{a + b}{2} - \left( \nu_n^{(2j)} - \frac{a + b}{2} \right).
\end{align*}
$$

**(B.2)**

It is furthermore possible to extend the construction of Leja knots to the case when $v_n \in \Gamma_\omega$ are Gaussian random variables (or more generally, random variables with a probability distribution other than uniform), see again [32, 57]. The knots thus obtained are the so-called Gaussian Leja knots (or in general, weighted Leja knots) and can be computed again recursively, by suitably introducing a weight in Equation (B.1), i.e., solving

$$
\nu_n^{(j)} = \arg\max_{v_n \in \Gamma_\omega} \sqrt{\rho_\omega(v_n)} \prod_{k=1}^{j-1} |v_n - v_n^{(k)}| ,
$$

where $\rho_\omega$ is the PDF of the random variable. Symmetric versions of Gaussian (weighted) Leja points can then be generated following the procedure that leads to Equation (B.2).

**References**

[1] Ian Gibson, David W Rosen, Brent Stucker, Mahyar Khorasani, David Rosen, Brent Stucker, and Mahyar Khorasani. *Additive Manufacturing Technologies*, volume 17. Springer, 2021.

[2] Wayne E King, Andrew T Anderson, Robert M Ferencz, Neil E Hodge, Chandrika Kamath, Saad A Khairallah, and Alexander M Rubenchik. Laser powder bed fusion additive manufacturing of metals; physics, computational, and materials challenges. *Applied Physics Reviews*, 2(4):041304, 2015.

[3] Sohini Chowdhury, N Yadaiah, Chander Prakash, Seeram Ramakrishna, Saurav Dixit, Lovi Raj Gulta, and Dharam Buddha. Laser powder bed fusion: A state-of-the-art review of the technology, materials, properties & defects, and numerical modelling. *Journal of Materials Research and Technology*, 2022.

[4] Jacob Smith, Wei Xiong, Wentao Yan, Stephen Lin, Puikei Cheng, Orison L Kafka, Gregory J Wagner, Jian Cao, and Wing Kam Liu. Linking process, structure, property, and performance for metal-based additive manufacturing: Computational approaches with experimental support. *Computational Mechanics*, 57(4):583–610, 2016.

[5] Wayne King, Andrew T Anderson, Robert M Ferencz, Neil E Hodge, Chandrika Kamath, and Saad A Khairallah. Overview of modelling and simulation of metal powder bed fusion process at lawrence livermore national laboratory. *Materials Science and Technology*, 31(8):957–968, 2015.

[6] Mohamad Bayat, Wen Dong, Jesper Thorborg, Albert C To, and Jesper H Hattel. A review of multi-scale and multi-physics simulations of metal additive manufacturing processes with focus on modeling strategies. *Additive Manufacturing*, 47:102278, 2021.
behavior, surface topography, and dendritic microstructure in selective laser melting of inconel 625. *Integrating Materials and Manufacturing Innovation*, 8(2):178–193, 2019.

[41] Bhanuprakash Sairam Kosaraju. *Prediction of Residual Stress and Distortion in Laser Powder Bed Fusion Additive Manufacturing*. PhD thesis, University of South Carolina, 2021.

[42] Yiğit M Arısoy, Luis E Criales, and Tuğrul Özal. Modeling and simulation of thermal field and solidification in laser powder bed fusion of nickel alloy in625. *Optics & Laser Technology*, 109:278–292, 2019.

[43] Chao Li, Erik R Denlinger, Michael F Gouge, Jeff E Irwin, and Pan Michaleris. Numerical verification of an octree mesh coarsening strategy for simulating additive manufacturing processes. *Additive Manufacturing*, 30:100903, 2019.

[44] Kyung-Min Hong, Corbin M Grohol, and Yung C Shin. Comparative assessment of physics-based computational models on the nist benchmark study of molten pool dimensions and microstructure for selective laser melting of inconel 625. *Integrating Materials and Manufacturing Innovation*, 10(1):58–71, 2021.

[45] Alfio Quarteroni, Riccardo Sacco, and Fausto Saleri. *Matematica Numerica*. Springer Science & Business Media, 2010.

[46] Ilya M Sobol. Global sensitivity indices for nonlinear mathematical models and their monte carlo estimates. *Mathematics and computers in simulation*, 55(1-3):271–280, 2001.

[47] A. Saltelli, M. Ratto, T. Andres, F. Campolongo, J. Cariboni, D. Gatelli, M. Saisana, and S. Tarantola. *Global Sensitivity Analysis: The Primer*. Wiley, 2008.

[48] B. Sudret. Global sensitivity analysis using polynomial chaos expansions. *Reliability Engineering and System Safety*, 93(7):964 – 979, 2008.

[49] L. Formaggia, A. Guadagnini, I. Imperiali, V. Lever, G. Porta, M. Riva, A. Scotti, and L. Tamellini. Global sensitivity analysis through polynomial chaos expansion of a basin-scale geochemical compaction model. *Computational Geosciences*, 17(1):25–42, 2013.

[50] Steve Brooks, Andrew Gelman, Galin Jones, and Xiao-Li Meng. *Handbook of Markov Chain Monte Carlo*. CRC press, 2011.

[51] Emanuel Parzen. On estimation of a probability density function and mode. *The Annals of Mathematical Statistics*, 33(3):1065–1076, 1962. ISSN 00034851.

[52] Murray Rosenblatt. Remarks on some nonparametric estimates of a density function. *The Annals of Mathematical Statistics*, 27(3):832–837, 1956. ISSN 00034851.

[53] A. Haji-Ali, P. Nobile, L. Tamellini, and R. Tempone. Multi-index stochastic collocation for random PDEs. *Computer Methods in Applied Mechanics and Engineering*, 306:95–122, 2016.

[54] C. Piazzola, L. Tamellini, R. Pellegrini, R. Breglia, A. Serani, and M. Diez. Comparing Multi-Index Stochastic Collocation and Multi-Fidelity Stochastic Radial Basis Functions for Forward Uncertainty Quantification of Ship Resistance. *Engineering with Computers*, 2022. doi: 10.1007/s00366-021-01588-0.

[55] John D. Jakeman, Michael Eldred, Gianluca Geraci, and Alex Gorodetsky. Adaptive multi-index collocation for uncertainty quantification and sensitivity analysis. *International Journal for Numerical Methods in Engineering*, 121(6):1314–1343, 2020.

[56] Grzegorz W Wasilkowski and Henryk Woźniakowski. Explicit cost bounds of algorithms for multivariate tensor product problems. *Journal of Complexity*, 11(1):1–56, 1995.

[57] Akil Narayan and John D. Jakeman. Adaptive Leja Sparse Grid Constructions for Stochastic Collocation and High-Dimensional Approximation. *SIAM Journal on Scientific Computing*, 36(6):A2952–A2983, 2014.