My suggestion for title: “Fast Surrogate Modeling with High-Dimensional Input and Output: Application to Additive Manufacturing” (I am not sure whether the second part is necessary. Let us talk about this.)

Also, we need to add Tina Lee from NIST as co-author; this is needed for NIST grants.

%% ABSTRACT

\section\*{Abstract}

An efficient approach referred to as the PCAS method for surrogate modeling in the presence of high-dimensional input and output is

proposed. Specifically, a large

collection of input variables is mapped to an output of interest which is a field quantity as opposed to a scalar.

Computational efficiency is accomplished by first identifying principal components~(PC)

or directions in the output field data. A set of representative features corresponding to the important directions of the high-dimensional output is

determined. A map from the set of inputs in the physical space to each feature is considered,

and the active subspace~(AS) methodology is used to capture their relationship in a low-dimensional subspace in the input

domain. The map for each feature of the output is then approximated by a surrogate in the active subspace. Thus, the PCAS

method aims at \textit{compounded} dimension reduction in both the input and the output. The resulting map is referred to as the \textit{composite surrogate}.

The proposed framework is implemented to build a surrogate for the purpose of reliability analysis with respect to

residual stress in an additively

manufactured component. The surrogate is further exploited for detecting

stress hotspots in the component, and for global sensitivity analysis to determine the impact of process variables and

alloy material properties on the development of residual stress. Our findings based on the considered application

are indicative of enormous potential for computational gains for such analyses.

\bigskip

\noindent \textbf{Keywords}: Principal components, active subspace, surrogate model, dimension reduction,

residual stress, additive manufacturing

%%% INTRODUCTION

\section{Introduction}

\label{sec:intro}

A surrogate model can offer a significant computational advantage in situations involving

intensive simulations, especially for applications

involving a large number of model evaluations such as uncertainty propagation, sensitivity analysis, parameter

estimation, and optimization. However, constructing a reasonably accurate surrogate itself can be computationally demanding.

For instance, estimation of coefficients of a polynomial chaos expansion (PCE)~\cite{Xiu:2002,Ghanem:1991},

a commonly used surrogate

in scientific applications, suffers from the so-called `curse of dimensionality'. Although remarkable progress has been

made towards efficient computation of the PC coefficients~(e.g. sparse

grids~\cite{Gerstner:1998,Ganapathysubramanian:2007} and basis adaptive

methods~\cite{Blatman:2011,Conrad:2013,Winokur:2013}), it remains computationally challenging for high-dimensional

applications especially if the output quantity of interest~(QoI) is a field as opposed

to a scalar quantity. Similarly, in the case of Gaussian

Process~\cite{Rasmussen:2004} surrogate modeling, computing the inverse of the correlation matrix becomes challenging in large dimensions. The complexity of

a neural network is also expected to increase with dimensionality and consequently, the training process requires a large

amount of data.

\*\*\* Need a literature review on surrogate modeling for multi-variate output, and for high-dimensional inputs and outputs \*\*\*\*\*

\*\*\* Need literature review on low-dimensional structure discovery. Active subspace is one method, manifolds is another; there may be other methods \*\*\*\*\*

In this paper, we develop a novel approach to surrogate modeling that focuses on combining the dimensionality reduction in the \textit{output}

space wherein the observation is a field quantity (as opposed to scalar) with dimensionality reduction in the \textit{input}

space. More specifically, we first exploit principal component analysis to extract key features in the output. Then, we

discover a

low-dimensional structure in the relationship between the output features and the set of inputs using the active

subspace methodology~\cite{Constantine:2015}. Hence, the proposed framework involves \textit{compounded} dimension

reduction wherein the dimension reduction is performed on key features of a field. The proposed methodology is

referred to as the PCAS method in this work as it combines principal components (PC) with active subspaces (AS).

The framework is implemented to

perform reliability analysis of an additively manufactured~(AM) part by assessing the development of residual stress

at the end of a single pass of a laser scan in electron beam melting (EBM).

Residual stress develops during the manufacturing process due to the presence of steep thermal gradients as

well as physical constraints in the part which adversely affect its mechanical properties, geometry, and

shape~\cite{Withers:2001,Mercelis:2006,Hofmann:2014}.

In fact, residual stress in addition to porosity is one of the main reasons for

part failure~\cite{Kim:2018}. The presence of residual stress in an AM part has significantly

inhibited rapid certification as well as standardization of the certification process

due to post processing involving machining and heat treatment~\cite{Shiomi:2004}.

Several recent investigations~\cite{Vastola:2016,Hodge:2016,Williams:2018}

have focused on developing thermo-mechanical

models to better understand the development of residual stress and optimize the microstructure as well as

the process control parameters accordingly. However, since the simulations are intensive and models require a

large amount of calibration data, the progress has so far been limited by the availability

of computational and experimental resources. Through this study, we aim to demonstrate an effective strategy

based on surrogate modeling that could accelerate material selection, microstructure design, and

process control and optimization for controlling the evolution of residual stress during additive manufacturing.

Since residual

stress is a field quantity and reliability analysis typically requires a large number of simulations, it is not practical

to rely on a finite element model (FEM) that could take hours per run. Additionally, conventional approaches for surrogate

modeling would require a large amount of computational resources for the purpose of training as discussed earlier.

A random field approximation is a possibility for

output dimension reduction. However, such an approximation could potentially introduce large errors in the

representation of the nonstationary output field. Instead, we aim to exploit the structure in the output data by identifying important

directions or principal components in the field. This approach allows us to select an optimal number of

features required to re-construct the field with reasonable accuracy and computational effort.

The key contributions of this paper can be summarized as follows: (1) A computationally efficient approach is developed

for constructing a surrogate model for problems where both the input and output are high-dimensional. (2) A finite element model is developed to simulate residual stress in an additively manufactured part

at the end of a single scan of the laser beam in an EBM process. (3) The surrogate is used to perform a global

sensitivity analysis~(GSA) to assess relative importance of the material properties and the process control parameters

in the context of residual stress. (4) Finally, the surrogate is used for the purpose of reliability analysis by estimating the

probability of failure using \textit{hotspot detection} in the part.

The remainder of this paper is organized as follows: Section~\ref{sec:method} outlines the proposed methodology for

constructing the surrogate model including a brief background on the active subspace methodology used in this work.

Section~\ref{sec:model} details the finite element model used to generate the stress data for building the surrogate.

Section~\ref{sec:results} provides numerical results and discussion pertaining to the implementation of the methodology

for surrogate construction, GSA, and reliability analysis of the AM product.

Finally, we summarize this study in Section~\ref{sec:conc}.

%%% METHOD

\section{Proposed PCAS Method}

\label{sec:method}

As discussed earlier in Section~\ref{sec:intro}, we aim to construct a surrogate for mapping the set of inputs to a

field quantity. In the proposed methodology, we outline a two-step process to accomplish this. The first step involves

dimension reduction in the output space that involves

identification of principal directions or components in the data set for the field of interest. These components are used

to construct a feature vector. Each element in the feature vector is an inner product of the field data and elements

of a given principal direction. Hence, the number of features is equal to the number of principal directions used to

reconstruct the field. In the second step, each feature is represented as a function of the inputs and a low-dimensional

representation of the function is computed

using the active subspace methodology outlined in~\cite{Constantine:2015}. The active subspace predominantly

captures the variability in each feature due to the variability in the inputs.

In~\ref{sub:pca}, we outline

the strategy for computing the feature vector. In~\ref{sub:as}, we provide a brief background on active subspaces

and outline the sequence of steps for surrogate construction for each feature.

\subsection{Principal Component Analysis}

\label{sub:pca}

For the purpose of outlining the computational framework, we consider a field,

$\mat{S}(\bm{\theta})\in\mathbb{R}^{r\times c}$ evaluated on a 2-dimensional mesh of size $r\times c$;

and $\bm{\theta}$ denotes the set of inputs. Consider that the field data is available at $N\_s$ pseudorandom

samples, drawn from the joint probability density function (pdf) of $\bm{\theta}$. A data matrix $\mat{X}$ is

first constructed using the field data at $N\_s$ samples. A singular value decomposition of the covariance

matrix, $\mat{X^\top X}$ is then performed to obtain an orthogonal matrix, $\mat{U}$ whose columns

contain eigenvectors or principal directions in the considered data. A matrix, $\mathcal{Z}$ with

rows as feature vectors corresponding to each

sample is obtained by multiplying the matrices, $\mat{X}$ and $\mat{U}$. The number of features

are thus equal to the number of components or columns considered in $\mat{U}$.

The field $\mat{S}$ can be reconstructed by multiplying $\mathcal{Z}$ and the transpose of $\mat{U}$

considering the latter is orthogonal.

Since most of the information is captured by the dominant eigenvectors, $\mat{S}$ can be re-constructed with a

reasonable amount of accuracy in a low-dimensional column space of $\mat{U}$. We adopt an iterative

approach wherein the number of eigenvectors or components of $\mat{U}$ are increased by one at each iteration

and the accuracy of the reconstructed field, $\hat{\mat S}$ is assessed. Thus, the optimal number of components

correspond to the reconstruction error~($\varepsilon\_\mathcal{R}^\infty$)

being smaller than a considered threshold, $\tau$. The sequence of steps

is outlined in Algorithm~\ref{alg:pca}.

%

\bigskip

\begin{breakablealgorithm}

\renewcommand{\algorithmicrequire}{\textbf{Input:}}

\renewcommand{\algorithmicensure}{\textbf{Output:}}

\caption{Determining the optimal number of components, $K^\ast$ for reconstructing $\mat{S}$}

\begin{algorithmic}[1]

\Require $\tau$, $\mat{S}\_i$'s, $\bm{\theta\_i}$'s ($i=1,2,\ldots,N\_s$)

\Ensure $\mat{U}^r$, $K^\ast$

\Procedure{Iterative PCA}{}

\State Construct the data matrix, $\mat X$:

\State Set $k$ = 0

\Loop

\State Reshape $\mat{S}\_i\in\mathbb{R}^{r\times c}$ into a vector,

$\vec{S}\_{v,i}\in\mathbb{R}^{(r\ast c)\times 1}$

\State $k=k+1$

\State $\mat X(k,:)=\vec{S}\_{v,i}$

\If {$k=N\_s$}

\State break

\EndIf

\EndLoop

\State Perform an SVD on the covariance matrix, $\mat{X}^\top \mat{X}$:

\Statex \[ \mat{X}^\top \mat{X} = USV^\top \]

\State Optimize the number of components, $K$:

\State Set $K$ = 1

\Loop

\State Compute the feature matrix, $\mat{\mathcal{Z}}$:

\[ \mat{\mathcal{Z}} = \mat{X}\mat{U}(:,1:K) \]

\State Reconstruct the field, $\mat{S}$ as $\hat{\mat{S}}$:

\[ \hat{\mat{S}} = \mat{\mathcal{Z}}\mat{U}(:,1:K)^\top \]

\State Estimate the maximum error, $\varepsilon\_\mathcal{R}^\infty$:

\[ \varepsilon\_\mathcal{R}^\infty = \max\limits\_i \|\mat{S}\_i-\hat{\mat{S}}\_i\|\_\infty,~i=1,2,\ldots,N\_s\]

\If {$\varepsilon^\infty < \tau$}

\State $K^\ast = K$

\State $\mat{U}^r = \mat{U}(:,1:K^\ast)$

\State break

\EndIf

\EndLoop

\EndProcedure

\end{algorithmic}

\label{alg:pca}

\end{breakablealgorithm}

\bigskip

%

At the end of the iterative procedure, a feature vector with $K^\ast$ components is obtained for each $\bm{\theta\_i}$.

Dimension reduction in the output space is thus achieved since $K^\ast\ll (r\ast c)$, where $(r\ast c)$ is the

dimensionality of the column space of $\mat{U}$.

The feature matrix, $\mat{\mathcal{Z}}$ can be mathematically represented as follows:

\be

\mat{\mathcal{Z}} =

\begin{pmatrix}

\mathcal{Z}\_{11} & \mathcal{Z}\_{21} & \cdots & \mathcal{Z}\_{K^\ast 1} \\

\mathcal{Z}\_{12} & \mathcal{Z}\_{22} & \cdots & \mathcal{Z}\_{K^\ast 2} \\

\vdots & \vdots & \ddots & \vdots \\

\mathcal{Z}\_{1N\_s} & \mathcal{Z}\_{2N\_s} & \cdots & \mathcal{Z}\_{K^\ast N\_s}

\end{pmatrix}

\label{eq:feature}

\ee

%

The data matrix in the RHS of~\eqref{eq:feature} is used to construct an active subspace for each feature,

$\mathcal{Z}\_{i}$~($i$~=~$1,2,\ldots,K^\ast$) as discussed in the following section.

\subsection{Active Subspace Discovery}

\label{sub:as}

A given feature, $\mathcal{Z}\_{i}$ = $\mathcal{Z}\_{i}(\vec{\theta})$ can be considered as a scalar valued function

of the set of inputs, $\bm{\theta}$. An active subspace in the present context is a low-dimensional subspace in the input

domain that effectively captures the variability in $\mathcal{Z}\_{i}$ due to variations in $\bm{\theta}$.

The set of inputs, $\bm{\theta}$ in the physical space

are parameterized as canonical random variables, $\bm{\xi}\in\Omega\in\mathbb{R}^{\Nt}$, where $N\_\theta$

denotes the number of uncertain parameters referred to as the dimensionality of the parameter space. The active

subspace is spanned by the dominant eigenvectors of a matrix, $\mathbb{C}$ comprising the derivative information

of $\mathcal{Z}\_{i}$ with respect to the components of $\bm{\xi}$. Note that a component $\xi\_k$ can be projected back

to the physical space to its corresponding potential parameter, $\theta\_k$. The positive semi-definite matrix,

$\mathbb{C}$ for the $i^\text{th}$ feature is given as follows:

%

\be

\mathbb{C}\_i = \int\_\Omega (\nabla\_{\vec{\xi}}\mathcal{Z}\_{i})(\nabla\_{\vec{\xi}}\mathcal{Z}\_{i})^\top dP\_\vec\xi,

\label{eq:C}

\ee

%

where $dP\_\vec\xi$ = $\pi\_\vec\xi d\vec\xi$ and $\pi\_\vec\xi$ denotes the joint pdf of $\bm{\xi}$. Note that

$\mathcal{Z}\_{i}$ is assumed to be differentiable and L$^2$ integrable in $\Omega\_\theta$.

Since the integral in~\eqref{eq:C}

is multidimensional, the symmetric and positive semidefinite matrix $\mathbb{C}\_i$ is approximated numerically in

practice. Consider its sampling based estimate and associated eigenvalue decomposition as follows:

%

\be

\mathbb{C}\_i\approx \hat{\mathbb{C}}\_i = \frac{1}{N}\sum\limits\_{l=1}^{N}

(\nabla\_{\vec{\xi}}\mathcal{Z}\_{i}(\vec{\xi}\_l))(\nabla\_{\vec{\xi}}\mathcal{Z}\_{i}(\vec{\xi}\_l))^\top

= \hat{\mat{W}}\hat{\mat{\Lambda}}\hat{\mat{W}}^\top.

\label{eq:chat}

\ee

%

The matrix $\hat{\mat{W}}$ comprises orthonormal eigenvectors as its columns, and $\hat{\mat{\Lambda}}$

is a diagonal matrix with eigenvalues arranged in descending order as its elements:

\[

\lambda\_1 \geq \lambda\_2 \geq \cdots \geq \lambda\_\Nt \geq 0.

\]

Dimension reduction is achieved by partitioning the eigenpairs about the $j^{\text{th}}$ eigenvalue

such that \scalebox{1.25}{$\left(\frac{\lambda\_j}{\lambda\_{j+1}}\right)$}$\gg 1$ as follows:

\be

\hat{\mat{W}} = [\hat{\mat{W}}\_1~\hat{\mat{W}}\_2],~~\hat{\mat{\Lambda}} = \begin{bmatrix}\hat{\mat{\Lambda}}\_1 & \\ &

\hat{\mat{\Lambda}}\_2.

\end{bmatrix}

\ee

%

The column space of $\hat{\mat{W}}\_1$ constitutes the active subspace, and $\hat{\mat{\Lambda}}\_1$ is the

corresponding diagonal matrix with its elements: $\{\lambda\_1,\ldots,\lambda\_\Nj\}$, where $\Nj$ is the number

of columns or eigenvectors in $\hat{\mat{W}}\_1$. $\mathcal{Z}\_{i}$,

a function of $\Nt$ independent variables is transformed as $G(\bm{\eta})$, a function of $j$ independent

variables since $\bm{\eta}=\hat{\mat{W}}\_1^\top \bm{\xi}\in\mathbb{R}^\Nj$. The components of $\bm{\eta}$

are referred to as \textit{active variables}.

From~\eqref{eq:chat}, it is clear that the computational effort needed to construct $\mathbb{C}\_i$ is directly proportional

to the number of samples, $N$. A regression-based approach outlined

in~\cite{Vohra:2019} was used to estimate the gradients of $\mathcal{Z}\_{i}$,

required to compute the elements of $\mathbb{C}\_i$.

\subsubsection{Surrogate in the Active subspace}

\label{sub:surr}

Significant computational gains are expected in situations where a low-dimensional active subspace captures the

variability in the output with reasonable accuracy. However, gains can be increased further by constructing a

surrogate ($\hat{G}(\bm{\eta})$) for the variability ($G(\bm{\eta})$) in the subspace. If the surrogate is 1- or 2- dimensional,

a simple polynomial regression fit might be adequate. However, for a relatively large dimensional surrogate, one could

use a PCE or a GP. It is critical to validate the surrogate for its predictive accuracy.

The following algorithm provides a sequence of steps adapted from~\cite{Constantine:2015} to construct a

surrogate in the active subspace.

%

\begin{breakablealgorithm}

\renewcommand{\algorithmicrequire}{\textbf{Input:}}

\renewcommand{\algorithmicensure}{\textbf{Output:}}

\caption{For constructing a surrogate model in the active subspace}

\begin{algorithmic}[1]

\Procedure{Surrogate Model, $\hat{G}(\bm{\eta})$}{}

\State Consider $N$ available data points in the full space, $(\vec\xi\_k,\mathcal{Z}\_i(\vec\xi\_k))$, $k~=~1,\ldots,N$

\State For each $\vec\xi\_k$, compute $\vec\eta\_k$ = $\mat{W}\_1^\top\vec\xi\_k$

(Note: $G(\vec{\eta}\_k)$ $\approx$ $\mathcal{Z}\_i(\vec{\xi}\_k)$)

\State Fit a regression surface, $\hat{G}(\bm{\eta})$ to approximate $G(\bm{\eta})$ using the data

points, $(\vec\xi\_k,G(\vec\eta\_k))$

\State Note that the overall approximation is: $\mathcal{Z}\_i(\vec{\xi})$ $\approx$

$\hat{G}(\mat{W}\_1^\top\vec{\xi})$

\EndProcedure

\end{algorithmic}

\label{alg:surr}

\end{breakablealgorithm}

%

To sum up, an active subspace is computed for each dominant feature, $\mathcal{Z}\_i$ and a corresponding

surrogate fit, $\hat{\mathcal{Z}}\_i$ is performed. Therefore, a total of $K^\ast$ surrogates are constructed

to map the set of inputs $\bm{\theta}$ in the physical space to the field in the output space. The overall dimension

reduction accomplished using the proposed methodology is $\mathbb{R}^{(r\ast c)}\rightarrow \mathbb{R}^{N\_{\bm{\eta},

\max}}$; where $N\_{\bm{\eta},\max}$ is the maximum number of active variables, $\bm{\eta}$ required to construct

a given $\hat{G}\_i$, i.e. $\max\limits\_j \Nj$. A overall flow diagram for the proposed methodology is provided in

Figure~\ref{fig:fd}.

%

\begin{figure}[htbp]

\begin{center}

\begin{tikzpicture}[node distance=1.2cm,scale=0.6, every node/.style={scale=1.0}]

\node (field) [io, text width=6em] {Field Data\\ $\mat{S}\in\mathbb{R}^N$};

\node (pca) [process, right of=field, text width=15em, xshift=7.5cm] {Optimal number of features: \\

$\mathcal{Z}\_i$, $i=1,\ldots,K^\ast$\\

DR: $\mathbb{R}^{N}\rightarrow \mathbb{R}^{K^\ast},~K^\ast\ll N$};

\draw [arrow] (field) -- node[above] {Principal Component} node [below] {Analysis} (pca);

\node (zk) [process, below of=pca, text width=8em, yshift=-3.0cm] {$\mathcal{Z}\_i=\mathcal{Z}\_i(\bm{\theta})$\\

$\bm{\theta}\in\mathbb{R}^{\Nt}$};

\draw [arrow] (pca) -- (zk);

\node (as) [io, below of=field, text width=16em, yshift=-3.0cm]{$\mathcal{Z}\_i(\bm{\theta})\approx

G(\bm{\eta}=\bm{\theta}^\top \bm{W\_1})$\\

$G(\bm{\eta})\approx \hat{G}(\bm{\eta})$, $\eta\in\mathbb{R}^{\Nj}$\\

DR: $\mathbb{R}^{\Nt}\rightarrow \mathbb{R}^{N\_{\bm{\eta},\max}}$, $N\_{\bm{\eta},\max}\ll \Nt$};

\draw [arrow] (zk) -- node [above] {Active Subspace} node [below] {Computation} (as);

\draw [arrow,dashed] (as) -- (field);

\end{tikzpicture}

\end{center}

\caption{Flow diagram illustrating the sequence of steps and associated dimension reduction (DR) in the PCAS method.}

\label{fig:fd}

\end{figure}

%

Once a surrogate for each feature is built, the field of interest can be reconstructed as shown in Figure~\ref{fig:re}.

%

%

\begin{figure}[htbp]

\begin{center}

\begin{tikzpicture}[node distance=1.2cm,scale=0.6, every node/.style={scale=1.0}]

\node (s1) [io, text width=7.5em] {Draw a sample, $\bm{\xi}\_k$ from $\pi\_\xi$};

\node (s2) [process, right of=s1, text width=8em, xshift=3.0cm] {Compute $\hat{G}\_i(\bm{\xi}\_k)$\\ $i=1,2,\ldots,K^\ast$};

\draw [arrow] (s1) -- (s2);

\node (s3) [process, right of=s2, text width=9em, xshift=3.0cm] {$\mathcal{Z}\_i(\bm{\xi}\_k)\approx\hat{G}\_i(\bm{\xi}\_k)$};

\draw [arrow] (s2) -- (s3);

\node (s4) [process, right of=s3, text width=7em, xshift=2.8cm] {Compute $\hat{\mat{S}}(\mathcal{Z}\_i)$};

\draw [arrow] (s3) -- (s4);

\end{tikzpicture}

\end{center}

\caption{Flow diagram illustrating the sequence of steps for reconstructing the field of interest.}

\label{fig:re}

\end{figure}

%%% MODEL

\section{Electron Beam Melting: Finite Element Model}

\label{sec:model}

Electron beam melting (EBM) is an additive manufacturing process of fusing powder particles, layer-upon-layer,

using an electron beam as the energy source. The process is typically used in the case of metals and its alloys.

Multiple passes of a low power electron beam is used for heating and sintering the powder bed prior to selective

melting. For the application problem in this study, we focus on the thermo-mechanical behavior of an AM part

produced by the EBM process. For this purpose, we have developed a finite element-based thermal analysis

model to simulate the thermal response of the part, and a finite element-based mechanical model that uses the part’s thermal

response to estimate the residual stress in the part at the end of the cooling phase. In this study, the two models are

weakly coupled, i.e. the temperature history of the part is used as an input heat load for the mechanical model.

Finite element analysis is performed using Abaqus~\cite{Hibbitt:2001}, a commercially available software.

Our analysis is based on stress development in an AM part as a result of a single scan of an

electron beam along its

length. A layer thickness, 50~$\mu$m and a part of dimensions (in mm), 2$\times 1.5\times 0.65$ is used as shown

in Figure~\ref{fig:PartwMesh}~(left).

The process of laying the new powder on bulk material formed by previous scans is simulated

by activating the initially deactivated elements representing the powder layer. To mitigate computational cost

associated with FEA, a non-uniform mesh is employed wherein a finer mesh is considered for the powder

region where the heat flux is applied. A gradually coarsening mesh is considered for the bulk material, significantly far

from the heat source as shown in Figure~\ref{fig:PartwMesh}~(right). The mesh consists of 13,200 nodes and

10,752 elements in total.

%

\begin{figure}[htbp]

\begin{center}

\includegraphics[width=0.4\textwidth]{./Figures/EBM\_PartwXYZ}

\includegraphics[width=0.4\textwidth]{./Figures/meshwXYZ}

\end{center}

\caption{Part geometry and the corresponding mesh as modeled in Abaqus}

\label{fig:PartwMesh}

\end{figure}

%

The material used to manufacture the part is considered to be Ti-6Al-4V and its

thermophysical properties considered in the FEM analysis are provided in Table~\ref{tab:matProp}.

%

\begin{table}[htbp]

\centering

\caption{Thermophysical properties of Ti-6Al-4V~\cite{Fu:2014}}

\label{tab:matProp}

\vspace{1mm}

\begin{tabular}{ ll }

\toprule

Density (kg $/$m$^3$) & 4428\\

Solidus Temperature ($^\circ$ C) & 1605 \\

Liquidus Temperature ($^\circ$ C) & 1655\\

Latent heat (J$/$kg) & 365000\\

Elastic Modulus (GPa) & 110 \\

Poisson's ratio & 0.41\\

Yield strength (MPa) & 825\\

\bottomrule

\end{tabular}

\end{table}

%%%

\subsection{Thermal Model}

\label{sub:thermal}

The governing equation for the heat transfer analysis \cite{Zinoviev:2016} is given by:

\begin{equation}\label{eq\_thermal}

\rho {C\_p}\frac{{\partial T}}{{\partial t}} = -\nabla\cdot ({\kappa}\nabla T) + Q\_e - Q\_r

\end{equation}

where $T$, $\rho$, $C\_p$, $\kappa$, $Q\_e$ denote the local temperature, average density, specific heat, thermal conductivity,

and the applied heat flux respectively. A single scan is considered along the x-direction at the top surface of the part.

The moving electron beam heat source is modeled as a Gaussian~\cite{Vastola:2016} according to the following

equation:

%

\begin{equation}\label{eq\_heatFlux}

Q\_e = \frac{2P}{\pi r^2 d}e^{\frac{-2((x-vt)^2+y^2)}{r^2}}\frac{1}{5}\Big[-3\Big(\frac{z}{d}\Big)^2-2\frac{z}{d}+5\Big]

\end{equation}

%

where $P=\alpha IV$ denotes the power associated with the electron beam for a given absorptivity~($\alpha$),

current~(I), and voltage~(V). The quantities: $v$, $r$, and $d$ denote the beam velocity or scan speed,

beam spot radius, and penetration depth respectively. The external heat source is illustrated using temperature

contours on the top surface in Figure~\ref{fig:thermal}~(left) and along x-z plane passing through the center of the part in

Figure~\ref{fig:thermal}~(right).

%

\begin{figure}[htbp]

\begin{center}

\includegraphics[width=0.42\textwidth]{./Figures/NT11Nom3D}

\includegraphics[width=0.42\textwidth]{./Figures/NT11Nom}

\end{center}

\caption{Left: Temperature contours associated with the moving electron beam as a heat source. Right:

Temperature contours in the x-z plane passing through the center of the part once the electron beam is

turned off.}

\label{fig:thermal}

\end{figure}

%

The laser beam radius~($r$) and the thermal penetration depth are fixed at 200 and 28

microns respectively. The powder is pre-heated to a temperature, $T\_0$ prior to the scan using fixed temperature

boundary conditions at the lateral sides as well as the bottom of the part. Heat transfer in the part occurs by two

mechanisms: First, by means of thermal conduction due to temperature gradients especially along the depth (x-z plane),

and second, by means of radiative losses from the exposed surface of the part denoted as $Q\_r$ in~\eqref{eq\_thermal}.

The radiative heat flux, $Q\_r$ is modeled using the Stefan-Boltzmann law i.e., $Q\_r=\sigma\epsilon(T^4-T\_a^4)$, where

$\sigma$, $\epsilon$, and $T\_a$ denote the Stefan-Boltzmann constant, emissivity of the top surface, and the ambient

temperature respectively. Note that convective losses are not considered since the manufacturing process is assumed to be

carried out in vacuum. As discussed later in Section~\ref{sec:results}, the laser beam power~($P$), scan speed~($v$), and

pre-heat temperature of the powder bed~($\theta\_0$) are considered as process control parameters~($\bm{\theta\_p}$)

in our analysis using the surrogate model. The temperature history of the part determined using the thermal model

is used as an input to the mechanical model (one way coupling) to compute residual stress in the AM part as

discussed in the following section.

\subsection{Mechanical Model}

\label{sub:mech}

The governing equation for structural analysis \cite{Megahed:2016} is given by:

%

\begin{equation}\label{eq\_mechanical}

\nabla \cdot \mat{\sigma}+f = 0

\end{equation}

%

where $\sigma$ and $f$ denote the stress tensor and the internal forces respectively. From Hooke's law, the stress

tensor ($\mat{\sigma}$) is proportional to the total strain~($\epsilon^T$). Material stiffness tensor, $\mat{C}$ is the

proportionality constant. The constitutive relationship is given as follows:

%

\be

\mat{\sigma} = \mat{C}\epsilon^T

\ee

%

where $\epsilon^T = \epsilon^e + \epsilon^p+ \epsilon^t$; $\epsilon^e$, $\epsilon^p$, and $\epsilon^t$ denote elastic,

plastic, and thermal strains respectively. The plastic strain is modeled by considering elastic

perfectly-plastic~\cite{Zhao:2015} condition in the model. Thermal strain is calculated from the thermal expansion

constitutive relationship: $\varepsilon^T = \alpha\_{t}\Delta T$, where $\alpha\_t $ is the thermal expansion coefficient.

The boundary surfaces in the X-direction and Y-direction are constrained in the x-

coordinates and y-coordinates respectively. The bottom surface is considered fixed in all coordinates.

Temperature history at each node, obtained using the thermal model in~\ref{sub:thermal}, is used to

compute the strain tensor, $\sigma$. Hence, the mechanical model is dependent on the thermal response

of the part but not vice versa. The coupling between the two models is therefore regarded as \textit{one-way}

or \textit{weak}~\cite{Debroy:2017}. Weak coupling between the models is essentially considered due to the fact

that a strong coupling would be computationally expensive. The von Mises stress at the end of the cooling process

is considered as the residual stress in the AM part. It is considered as the output quantity of interest~(QoI) in our analysis for

demonstrating the methodology proposed earlier in Section~\ref{sec:method}. The stress contours are illustrated

in Figure~\ref{fig:subSmises}

%

\begin{figure}[htbp]

\begin{center}

\includegraphics[width=0.6\textwidth]{./Figures/SMisesNom}

\end{center}

\caption{von Mises stress contours in the x-z plane passing through the center of the part after it has cooled

down to the ambient temperature.}

\label{fig:subSmises}

\end{figure}

%

The contour plot in Figure~\ref{fig:subSmises} clearly indicates that the residual stress in the part attains higher

values near the top surface and diminishes quickly along the depth of the part. It can thus be said that thermal

strain due to the applied heat flux is the dominant contributor to the residual stress in the present set-up.

Simulations are performed on a workstation with a system configuration: Intel~Core~i7-4790~CPU,

3.60 GHz with 16GB RAM. It is observed that on average the thermal model takes 20 minutes to complete a run, and the

mechanical model takes 10 minutes. Note, however, that the simulation duration depends on the choice of

values for the set of inputs.

%%% RESULTS

\section{Results}

\label{sec:results}

In this section, we provide relevant details pertaining to the construction of the surrogate model to predict the field quantity of interest, i.e. the

residual stress in the AM part cross-section using the PCAS method in~\ref{sub:surr}. The surrogate is used to map

the process control parameters and the material properties to the residual stress field. The computational efficiency

enabled by the surrogate is exploited to perform a global sensitivity analysis of the inputs in~\ref{sub:gsa}. Finally, the

surrogate is used for reliability prediction for the AM part by estimating the probability of failure based on residual stress

in~\ref{sub:reliability}.

\subsection{Surrogate Model}

\label{sub:surr}

A surrogate model is constructed for the residual stress field at the cross-section of the part

(x-z plane in Figure~\ref{fig:PartwMesh}) passing through its center. We will refer to this plane

as x$^c$-z$^c$ in the remainder of this paper. The surrogate maps three sets of

parameters, namely, the process control parameters~($\bm{\theta\_P}$), mechanical properties~($\bm{\theta\_M}$),

and thermal properties~($\bm{\theta\_T}$) to the stress field. The set of process control parameters includes

the beam power~($P$), scan speed~($v$), and the pre-heat temperature~($T\_0$). Mechanical properties

include the yield strength~($Y$), the elastic modulus~($E$), and the bulk density~($\rho$). Thermal

properties include specific heat~($C\_p$) and bulk thermal conductivity~($\kappa$). Note that $C\_p$ and $\kappa$

are considered to be functions of the local temperature, $T$. Specifically, a polynomial of degree 2 was fit

to a set of data pertaining to the variation of $C\_p$ and $\kappa$ with temperature (20~K--1655~K),

provided in~\cite{Fu:2014} as shown in Figure~\ref{fig:Cp\_kappa}.

%

\begin{figure}[htbp]

\begin{center}

\includegraphics[width=0.42\textwidth]{./Figures/cp\_fit}

\includegraphics[width=0.42\textwidth]{./Figures/kappa\_fit}

\end{center}

\caption{A second degree polynomial fit to specific heat~($C\_p$), and thermal conductivity~($\kappa$) data

for a temperature range, [20,1655](K). Note that the data provided in~\cite{Fu:2014} was used to determine

the coefficients of the regression fit.}

\label{fig:Cp\_kappa}

\end{figure}

%

Hence, a total of 12 parameters~($\bm{\theta}$) are mapped to the stress field including coefficients of the polynomial fits

corresponding to $C\_p$ and $\kappa$. A uniform prior: $[0.9\bm{\theta}^\ast, 1.1\bm{\theta}^\ast]$,

where $\bm{\theta}^\ast$ denotes a vector of nominal values,

is considered for each parameter. Nominal values of the mechanical properties: $Y$, $E$, and $\rho$ are provided

in Table~\ref{tab:matProp}. Nominal values of the process control parameters and temperature coefficients for

the thermal properties are provided in Table~\ref{tab:remain}.

%

\begin{table}[htbp]

\centering

\caption{EBM process control parameters and temperature coefficients for $C\_p$~($C\_i$'s) and $\kappa$~($D\_i$'s).}

\label{tab:remain}

\vspace{1mm}

\begin{tabular}{ ll }

\toprule

Scan Speed, $v$~(mm/s) & 500 \\

Beam Power, $P$~(W) & 160 \\

Pre-heat Temperature, $T\_0$~(C) & 650 \\

Specific heat, $C\_p$ = $C\_0+C\_1T+C\_2T^2$~(J/kg/K) & 540~($C\_0$),0.43~($C\_1$),$-3.2\times 10^{-5}$~($C\_2$) \\

Thermal Conductivity, $\kappa$ = $D\_0+D\_1T+D\_2T^2$~(W/m/K) & 7.2~($D\_0$),0.011~($D\_1$),$1.4\times 10^{-6}$~($D\_2$) \\

\bottomrule

\end{tabular}

\end{table}

%%%

Residual stress is computed at the x$^c$-z$^c$ plane for 20 pseudorandom samples in the 12-dimensional

input domain. Stress data is simulated on a 2-dimensional non-uniform grid comprising 32 points along the

length~(x$^c$) and 14 points along the height~(z$^c$) as highlighted in Figure~\ref{fig:RS\_comp}~(left).

As mentioned earlier in Section~\ref{sec:model}, a

finer mesh is used near the part surface since sharp thermal gradients lead to a larger amount of stress

in this region as shown in Figures~\ref{fig:subSmises} and~\ref{fig:RS\_comp}. Following the flow diagram

in Figure~\ref{fig:fd}, the first step involves a principal component analysis on the field data. For this purpose,

the iterative PCA algorithm~(Algorithm~\ref{alg:pca}) is used.

In Figure~\ref{fig:pca}, we plot the reconstruction error, $\varepsilon\_\mathcal{R}^\infty$ against the number of

principal components, $K$.

%

\begin{figure}[htbp]

\begin{center}

\includegraphics[width=0.42\textwidth]{./Figures/error\_PCA}

\end{center}

\caption{A plot of the reconstruction error, $\varepsilon\_\mathcal{R}^\infty$ as a function of the

number of principal components obtained using the iterative PCA approach in Algorithm~\ref{alg:pca}.}

\label{fig:pca}

\end{figure}

%

As expected, $\varepsilon\_\mathcal{R}^\infty$ is observed to mostly decrease with the number of components.

A monotonic behavior is not expected since the components only capture partial information in the data. It

appears that most of the information is captured using 20 components since the error is almost 0. However,

building the surrogate for 20 features would potentially entail a large computational effort depending upon the

application. Here, we consider that $K^\ast$ = 7 components are optimal since the error plateaus as the number of

components increase from 7 to 10 indicating diminishing returns. Thus, the residual stress field is reconstructed

using a surrogate for each of these $K^\ast$ components~($\mathcal{Z}\_i$'s, $i = 1,2,\ldots,K^\ast$).

The dimensionality of the output space is therefore reduced

from $\mathbb{R}^{14\times 32=448}\rightarrow \mathbb{R}^7$. We now shift our focus on dimension reduction

in the input space.

As discussed earlier in~\ref{sub:as}, each feature can be expressed as a function of $\bm{\theta}$ in the physical

space. Note that $\bm{\theta}:\{\bm{\theta\_P}\cup\bm{\theta\_M}\cup\bm{\theta\_T}\}$. An active subspace computation

was performed using a regression-based approach~\cite{Constantine:2015, Vohra:2019}

for estimating the gradient and the available set of 20 realizations for each $\mathcal{Z}\_i$.

The eigenvalue spectrum of the matrix, $\hat{\mathbb{C}\_i}$ for each $\mathcal{Z}\_i$ is shown in Figure~\ref{fig:as}.

The variability of a given $\mathcal{Z}\_i$ in terms of the active variables, $\bm{\eta}$ regarded as the sufficient summary

plot~(SSP) is also included in each case.

%

\begin{figure}[htbp]

\begin{center}

\begin{subfigure}{0.35\textwidth}

\includegraphics[width=0.65\textwidth]{./Figures/eig\_Zf1}

\\

\includegraphics[width=0.65\textwidth]{./Figures/eig\_Zf2}

\\

\includegraphics[width=0.65\textwidth]{./Figures/eig\_Zf3}

\\

\includegraphics[width=0.65\textwidth]{./Figures/eig\_Zf4}

\\

\includegraphics[width=0.65\textwidth]{./Figures/eig\_Zf5}

\\

\includegraphics[width=0.65\textwidth]{./Figures/eig\_Zf6}

\\

\includegraphics[width=0.65\textwidth]{./Figures/eig\_Zf7}

\end{subfigure}

\hspace{-0.5cm}

\begin{subfigure}{0.35\textwidth}

\includegraphics[width=0.65\textwidth]{./Figures/SSP\_Zf1}

\\

\includegraphics[width=0.65\textwidth]{./Figures/SSP\_Zf2}

\\

\includegraphics[width=0.65\textwidth]{./Figures/SSP\_Zf3}

\\

\includegraphics[width=0.65\textwidth]{./Figures/SSP2D\_Zf4}

\\

\includegraphics[width=0.65\textwidth]{./Figures/SSP\_Zf5}

\\

\includegraphics[width=0.65\textwidth]{./Figures/SSP\_Zf6}

\\

\includegraphics[width=0.65\textwidth]{./Figures/SSP\_Zf7}

\end{subfigure}

\end{center}

\caption{Eigenvalue spectrum and the corresponding SSP for each $\mathcal{Z}\_i$.}

\label{fig:as}

\end{figure}

%

From these plots, it is observed that in all cases except $\mathcal{Z}\_4$, a 1-dimensional active

subspace captures the variability in the feature with reasonable accuracy. More specifically, the

eigenvalue spectrum exhibits a significant jump between the first and second eigenvalue. Consistent

with these observations, a straight-line fit to the realizations of the feature in the SSP is observed to be

reasonably accurate. In the case of $\mathcal{Z}\_4$, $\lambda\_1$ and $\lambda\_2$ are comparable, and

a significant jump exists between $\lambda\_2$ and $\lambda\_3$. Therefore, a 2-dimensional active

subspace is considered. A polynomial regression surface fit is shown to capture the variability of

$\mathcal{Z}\_4$ with reasonable accuracy. Polynomials of degrees 3 and 2 along $\eta\_1$ and

$\eta\_2$ respectively were used to construct the regression surface. The regression-fits in each case

serves as a surrogate for the corresponding feature, $\mathcal{Z}\_i$. Therefore, a sample $\bm{\xi}\_i$

corresponding to $\bm{\theta}\_i$ in the physical space is propagated through each surrogate to estimate

$\mathcal{Z}\_i$'s and hence, the residual stress field as shown using a flow diagram in Figure~\ref{fig:re}.

The individual surrogates for $\mathcal{Z}\_i$'s thus constitute the overall surrogate model that maps the

physical input variables to the stress field. We will refer to this overall surrogate model as the \textit{composite

surrogate} in the remainder of this paper.

Dimension reduction in the input space is therefore found to be from $\mathbb{R}^7\rightarrow\mathbb{R}^2$.

The overall dimension reduction is therefore, $\mathbb{R}^{448}\rightarrow\mathbb{R}^2$ which indicates

enormous scope for computational gains using the PCAS method, and enables reliability prediction for the

AM part in a tractable manner.

\subsubsection{Surrogate Verification and Validation}

\label{subsub:vnv}

It is critical to \textit{verify} as well as \textit{validate} the accuracy of the resulting composite surrogate model

that maps variables in the physical space to the field of interest i.e., residual stress in the x$^c$-z$^c$ plane.

For verification, we reconstruct the stress field at the same set of 20 samples used to generate realizations

of the important features in the data for building the low-dimensional surrogate in each case. However, for the

purpose of validation, stress fields constructed at an independent set of 10 samples are compared to the

corresponding FEM predictions. To quantify the accuracy of the surrogate during verification and validation,

we compute an averaged relative L-2 error norm of the discrepancy~($\varepsilon\_d$) in the stress field, simulated using

the FEM and constructed using the surrogate model at the same set of grid points in the

2D mesh~(see Figure~\ref{fig:RS\_comp}~(left)). The mathematical expression for $\varepsilon\_d$ is given as

follows:

%

\be

\varepsilon\_{d} = \frac{1}{N}\sum\limits\_{i=1}^{N} \frac{\|\mat{S}-\hat{\mat{S}}\|\_2}{\|\mat{S}\|\_2},

\label{eq:test}

\ee

%

where, $N$ denotes the number of samples and is equal to 20 and 10 in the case of verification and validation

respectively; $\mat{S}$ and $\hat{\mat{S}}$ denote the stress field simulated using the FEM and the composite

surrogate respectively. The discrepancy error, $\varepsilon\_d$ was calculated to be approximately 0.04 and

0.07 in the case of verification and validation respectively. In other words, the stress field reconstructed using the

composite surrogate model achieves an accuracy of about 7$\%$ on average. Although these error estimates

are based on a relatively small sample size, they seem reasonable considering that the validation test samples

were generated using Latin hypercube sampling (LHS) that explores the entire input domain more uniformly

as compared to Monte Carlo sampling. Therefore, the PCAS approach appears to provide a reasonably

accurate (and simple) surrogate coupled with enormous computational gains which makes the sensitivity and reliability analyses pertaining to

the present application affordable.

Figure~\ref{fig:RS\_comp} illustrates a side-by-side comparison of stress distribution in the $x^c$-z$^c$ plane,

computed using the FEM~(left) with those generated using the composite surrogate~(right) using the same

set of input conditions. The two plots

are observed to be in close agreement with each other.

%

\begin{figure}[htbp]

\begin{center}

\begin{subfigure}{0.15\textwidth}

\vspace{10mm}

\includegraphics[width=0.5\textwidth]{./Figures/xczc}

\end{subfigure}

\hspace{-1.5cm}

\begin{subfigure}{0.35\textwidth}

\includegraphics[width=1.0\textwidth]{./Figures/origZ\_sam13}

\end{subfigure}

\hspace{0.25cm}

\begin{subfigure}{0.35\textwidth}

\includegraphics[width=1.0\textwidth]{./Figures/recZ\_sam13}

\end{subfigure}

\end{center}

\caption{Left: Residual stress field in the $x^c$-z$^c$ plane as generated using the Abaqus model with inputs,

$\bm{\theta}\_p$. The grid points in the 2D mesh used for finite element simulations are also highlighted.

Right: Reconstructed stress field using the surrogate model using: $v=535.23$~mm/s, $P$=148.27~W,

$T\_0$=641.03~K, $Y$=777.74~MPa, $E$=99.16~GPa, $\rho$=4187.25~kg/m$^3$, $C\_0$=546.43, $C\_1$=0.47,

$C\_2$~=~-~3.07$\times$10$^{-5}$, $D\_0$=6.84, $D\_1$=0.01, $D\_2$=1.47$\times$10$^{-6}$.}

\label{fig:RS\_comp}

\end{figure}

\subsubsection{Hotspot Detection}

\label{subsub:hotspot}

As mentioned earlier in Section~\ref{sec:intro}, a large amount of residual stress severely impacts part

performance due to sub-optimal mechanical properties, reduced fatigue life, and geometrical inaccuracy.

Detection of stress hotspots could thus be conceived as an important step in the manufacturing process.

Owing to the trasient nature of the process conditions, material microstructure, and part configuration,

it would not be practicable to use the FEM. The composite surrogate could instead be used for the purpose

of hotspot detection in the part.

For the present analysis, we focus on the hotspots in the $x^c$-z$^c$ plane, and any point in the 2D mesh

where the stress exceeds a threshold is considered as the hotspot. Figure~\ref{fig:hs} illustrates the

location of the hotspots and associated stress values in the $x^c$-z$^c$ plane, for a particular set of

input conditions. A threshold value of 640~MPa is used.

%

\begin{figure}[htbp]

\begin{center}

\includegraphics[width=0.42\textwidth]{./Figures/loc\_hotspot10}

\end{center}

\caption{Location of the hotspots in the AM part and corresponding estimates of the von Mises stress

are indicated by means of a colorbar. The location of the peak stress is also shown using a black square.}

\label{fig:hs}

\end{figure}

%

As expected, the hotspots are located near the top surface of the part that experiences sharp temperature

gradients.

\subsection{Global Sensitivity Analysis}

\label{sub:gsa}

The composite surrogate is next used for the purpose of global sensitivity analysis~(GSA). The residual stress

field in the $x^c$-z$^c$ plane is simulated for 10$^6$ pseudorandom samples, generating using LHS

in the 12-dimensional input domain. Thus, stress distribution is obtained at each point in the mesh.

The specific grid point with the maximum mean stress is regarded as the \textit{global hotspot},

denoted as P. Our findings reveal that P is in fact located at the top right corner of the $x^c$-z$^c$

plane, consistent with the location of the square in Figure~\ref{fig:hs}.

Figure~\ref{fig:kde\_S} shows the PDF of stress distribution at point P.

%

\begin{figure}[htbp]

\begin{center}

\includegraphics[width=0.42\textwidth]{./Figures/kde\_S\_mumax}

\end{center}

\caption{Probability density function~(PDF) of von Mises stress at location P, generated using kernel density estimation in

Matlab. The distribution is based on 10$^6$ evaluations and the mode value is estimated as 852.31~MPa.}

\label{fig:kde\_S}

\end{figure}

%

GSA is performed with respect to the stress value at point $P$.

As mentioned earlier, the set of inputs in the physical space, $\bm{\theta}$ is classified into three

categories: process control parameters~($\bm{\theta\_P}$), mechanical properties~($\bm{\theta\_M}$), and

thermal properties~($\bm{\theta\_T}$) of the alloy~(Ti6Al4V) used to manufacture the AM part. We focused

our efforts on determining the relative importance of $\bm{\theta\_P}$, $\bm{\theta\_M}$, and $\bm{\theta\_T}$

wherein the individual parameters in each category were grouped; and the relative importance of the process

control parameters and the material properties. The latter was performed by grouping $\bm{\theta\_M}$ and

$\bm{\theta\_T}$. GSA was performed by estimating the main-effect and the total-effect Sobol' sensitivity

indices at 10$^5$ samples in the input domain using an algorithm based on

Monte Carlo sampling~(MCS)~\cite{Sobol:2001}. The composite

surrogate was used to make the computations tractable. The estimated sensitivities for the two cases

are plotted in Figure~\ref{fig:gsa}.

%

\begin{figure}[htbp]

\begin{center}

\includegraphics[width=0.65\textwidth]{./Figures/grouped\_GSA}

\end{center}

\caption{Left: Sobol' sensitivity indices for the set of inputs grouped as process variables~($\bm{\theta\_P}:v,P,T\_0$),

mechanical properties~($\bm{\theta\_M}:Y,E,\rho$), and thermal properties~($\bm{\theta\_T}:C\_p,\kappa$).

Right: Sobol' sensitivity indices for the set of inputs grouped as process variables~($\bm{\theta\_P}$), and material

properties~($\bm{\theta\_{M,T}}$).}

\label{fig:gsa}

\end{figure}

%

Several inferences can be made: The residual stress at P is most sensitive to the mechanical properties, followed

by thermal properties of the alloy. Sensitivity towards the process control parameters is found to be relatively small.

However, it must be noted that the interactions between $\bm{\theta\_P}$, $\bm{\theta\_M}$, and $\bm{\theta\_T}$

are significantly large. Hence, the total-effect index of $\bm{\theta\_P}$ indicates that the sensitivity towards the

process variables is substantial. Therefore, optimizing the process parameters for minimizing residual

stress in the AM part could help improve its performance characteristics.

Note that these results are dependent on the choice of nominal values of the

inputs as well as the considered prior distribution in each case.

\subsection{Reliability Prediction}

\label{sub:reliability}

Reliability prediction involves estimating the probability of failure~($p\_f$) of the AM part

corresponding to a defined failure criterion. Here, we estimate~$p\_f$ based on the stress estimate at any location in

the part exceeding a given threshold. In other words, we aim to ensure that the residual stress

in the part does not exceed an upper bound and therefore, the performance characteristics of

the AM part are not severely degraded. Once again, we exploit the composite surrogate to

numerically estimate~$p\_f$ as follows:

%

\be

\hat{p}\_f = \frac{1}{N}\sum\limits\_{k=1}^{N} \mathbb{H}\left[S^\ast-\max(\hat{\mat{S}})\right],

\ee

\label{eq:pf}

%

where $\hat{p}\_f$ is the approximation to $p\_f$, $N$ denotes the number of samples, $S^\ast$

denotes the limiting stress value, and $\max(\hat{\mat{S}})$ denotes the peak stress in the

x$^c$-z$^c$ plane based on the surrogate prediction. $\mathbb{H}[]$

is a Heaviside unit step function that assumes a value 1 for a positive argument and 0 for

a negative argument.

To ensure that $\hat{p}\_f$ is a resonable approximation, it is estimated

using 10$^6$ samples in the input domain. Based on the generated samples, the probability of

failure using $S^\ast$~=~900~MPa is estimated to be 0.177.

%%% SUMMARY AND DISCUSSION

\section{Summary and Discussion}

\label{sec:conc}

In this paper, we have proposed an efficient approach, namely the PCAS method for constructing a surrogate model that

maps a high-dimensional input to a high-dimensional output. The high-dimensional output considered here is a field quantity,

estimated at discrete points on a mesh used for numerical simulations. Computational efficiency is

accomplished by means of dimension reduction in the output space as well as the input space.

We begin by determining the optimal number of

components required to reasonably approximate the output field using an iterative PCA approach~(Algorithm~\ref{alg:pca}).

Variability in each feature due to the variability

in the inputs is next captured in a low-dimensional subspace using the active subspace methodology. The PCAS method thus reduces the dimensionality

of the map from a set of inputs to key features in the output. Computational efficiency is enhanced by constructing

a surrogate in the active subspace computed for each feature. It is expected that the computational efficiency is accomplished with a trade-off in accuracy.

Therefore, it is critical to perform a robust verification and validation of the resulting surrogate model as discussed

in~\ref{subsub:vnv}.

The proposed methodology is demonstrated using an engineering application pertaining to reliability analysis of

an additively manufactured part. Specifically, we focused our efforts on predicting the development of residual

stress in a part at the end of an electron beam melting process using a finite element model in Abaqus.

The von Mises stress field in a 2-dimensional non-uniform mesh

in a cross-section of the AM part was computed, and it was found that

7 features were able to approximate the stress field using the iterative PCA approach. The set of inputs

comprising the process control parameters, mechanical and thermal properties of the alloy (used to manufacture the

AM part) were mapped to each of these 7 features. A 1- or 2- dimensional active subspace was shown to reasonably

capture the dependence of each feature on the inputs thereby indicating enormous scope for computational gains.

The surrogate was shown to be remarkably accurate by estimating the relative L-2 norm of the discrepancy

between the model output and the field reconstructed using the composite surrogate. Specifically, on average, the

surrogate achieved an accuracy of about 4$\%$ and 7$\%$ in the verification and validation tests respectively.

The surrogate was used to detect hotspots in the AM part~(Section~\ref{subsub:hotspot}), and to perform global sensitivity

analysis of the process variables, mechanical, and thermal properties of the alloy~(Section~\ref{sub:gsa}).

The hotspots were observed to be in the proximity of the applied heat source, i.e. closer to the surface of the

AM part, thereby indicating that the residual stress is dominated by the presence of large temperature gradients.

The GSA results

indicate that the residual stress is relatively more sensitive to the material properties, although the sensitivity

towards the process variables is also found to be significant due to their interactions with the material properties,

accounted for in the total-effect index. Finally, the composite surrogate was exploited to numerically estimate the

probability of failure using a million samples in the input domain for the purpose of reliability analysis of the AM part.

It must be highlighted that the aforementioned

analyses such as hotspot detection, GSA, and reliability prediction under various process and material uncertainties are typically computationally intensive in additive manufacturing.

The composite surrogate constructed using the PCAS method makes them computationally

affordable while ensuring a reasonable amount of accuracy for the present application.

However, there are limitations that should be considered

when applying the proposed framework. First, dimension reduction in the output space is conditioned upon the

existence of a structure in the data that could be captured by a relatively small number of principal components or

directions. Second, a low-dimensional active subspace is used here to map the set of inputs to the quantity of

interest~(QoI).

To accomplish this effectively, the gradient of the QoI with respect to each input should be estimated

with reasonable accuracy. For the application presented in this work, we have used a regression-based approach for

estimating the gradients that resulted in a reasonably accurate surrogate for each feature of the output field of interest.

However, depending upon the relationship between the QoI and the set of inputs, a relatively more accurate (but expensive) approach

such as those involving perturbation techniques~(e.g.~automatic differentiation~\cite{Kiparissides:2009}, adjoint

methods~\cite{Borzi:2011, Alexanderian:2017}) may be required. Additionally, the active subspace methodology is

not suitable in situations where the gradient is not continuous in the entire domain of the inputs.

To sum up, the proposed methodology was successfully demonstrated in this paper for a reasonably challenging practical

application involving reliability analysis of an additively manufactured part.

Enormous computational gains leading to dimension reduction by two orders of magnitude was accomplished. Therefore,

the proposed framework appears to be quite promising for surrogate building in applications involving large input and

output dimensions. Our future efforts will focus on further development of the proposed framework to enhance its

applicability as a prognosis tool for process control and optimization as well as defect characterization and minimization in

additive manufacturing.

%%% ACKNOWLEDGMENT

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