HDF5 Hierarchies for Additive Manufacturing digital representations and Enhanced Analytics

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Abstract

Advancement in Additive Manufacturing (AM) technologies and data acquisition techniques have led to an increase in AM data generated. However, due to the large volume and the diversity of AM data available it is becoming challenging to efficiently store, analyze, and represent AM processes. HDF5 has the potential to allow an easy access to big data by offering a hierarchical data catalog. Thus, AM processes could be represented through a hierarchy based on the data analytic needs and directly link the corresponding AM data.
This paper investigates the use of data formats to represent big data and AM dataset. Existing AM ontologies and models are reviewed in order to effectively encapsulate AM information and incorporate the hierarchy into an HDF5 AM wrapper. Three hierarchies are proposed to represent specific perspectives of AM processes: the digital twin of AM Product Lifecycle, the AM V model representation, and the material centric characteristics.

I. Introduction

Additive Manufacturing (AM), also referred to as 3D Printing, is a manufacturing process that allows the construction of parts layer-by-layer from a 3D model using specific techniques [1]. Multiple stages have been identified to represent the AM product lifecycle, the design, process plan, build, post process, test and validation [2]. Each stage generates large amounts of data with various types based on the corresponding stage's needs. Intensive experiment-based studies can be conducted in order to insure part quality and utilize the full potential of AM processes. However, it can be time consuming and costly [3]. Therefore, computational models and simulation have been developed to help part qualification by realizing process digitalization.

Hierarchical Data Format (HDF5) has been recently applied in different domains in order to help manage big datasets. In astronomy, Pourmal et al. uses HDF5 in order to store and quickly access huge astronomical dataset with earth science [4]. NASA has been using HDF5 in order to store images and radio frequency data from their Earth Observing System (EOS) [5]. In Biology, Dougherty et al. uses HDF5 in order to store huge dataset of biological images [6]. Jackson et al. developed an HDF5 model to support multi-dimensional datasets [7]. BioHDF is a HDF5 hierarchy that has been developed in order to represent and store experimental data [8]. In construction, Krijnen et al. have worked on translating the IFC standards for buildings in HDF5 [9]. A parser has been developed using the EXPRESS [10] syntax of Industry Foundation Classes (IFC) files [11] to automatically translate an IFC file and store it in a HDF5 file. In Manufacturing, Khan et al. uses HDF5 as a neutral format to allow the transfer of information between Computer Aided Design (CAD) et Computer Aided Engineering (CAE) [12]. Schmitz et al. have introduced Dream3D in order to model and represent in standardized and unique way microstructure [13]. All these different domains have proven the benefit and efficiency of using HDF5 format in order to easily store and manage big datasets. AM generates big data sets during the different processes and such format could help solve AM data challenges.

In this paper, the goal will be to improve AM process digitalization and data analysis by proposing an approach to help manage the large amounts of data generated from the different stages of the AM processes. The paper starts by introducing background work on data management to help organize and effectively improve AM computational efforts. We highlight the AM data challenges and describe the drive to develop better data organization. Then, we propose an approach that uses hierarchical data format in order to optimize data curation

and enhance data analytics. Finally, we showcase our approach by demonstrating the use of HDF5 as a base for digital twin implementation.

II. Hierarchical Organization of AM Data

1. Data Management to Drive AM Data Analysis

In order to efficiently use and store big datasets, three different types of data management techniques have been identified : based on model, based on ontology, and based on hierarchy.

Traditional databases are majorly used to maintain and store data in a specific format using a centralized architecture. Each database is described by a schema based on a model representing the system and the dataset. Lu et al. developed the Additive Manufacturing Integrated Data Model (AMID) in order to capture, store, and properly manage AM data for easy query and analysis [14]. This model has been created using the Product, Process, Resource (PPR) method and is used to represent the data in the Additive Manufacturing Material Database (AMMD). This traditional method of storing data is a good and proven way to represent datasets but it hardly supports big data, and doesn't allow for easy transfer of databases. A flat structure is used to describe heterogeneous datasets and doesn't allow for easy linkage of the data. Thus, the handling of big and complex datasets containing product lifecycle data is challenging and time-consuming. New concepts and data management methods have been investigated in order to bridge these challenges.

An ontology, in computer science, is a data model that represents a set of concepts within a domain and the relationships between those concepts. Antoniou et al. define ontology as "languages that allow users to write explicit, format conceptualizations of domain models" [15]. It allows to semantically describe a system, and represent it into a model that could then be fed with data generated by the system. Entities can then be stored based on the ontology model which creates a database that could easily be accessed and read by humans thanks to its structure. In additive manufacturing there have been several efforts working on ontology to represent the AM processes. There are different ways to define the AM processes either trying to describe the entirety of the AM processes [16, 17] or either focusing a specific analysis of the AM processes in order to orient the model [18, 19]. Sanfilippo et al. focused on developing an ontology in order to represent the AM product lifecycle. They aim to describe all the AM processes that would result in the creation of the physical part [20]. Samyeon at al. focused on developing an ontology that would focus on describing the data in order to support manufacturability analysis. This ontology is oriented in a way that it would be easier to determine the manufacturability of a part based on the data of the AM processes [21].

Hierarchical data formats (HDF5) consists of a hierarchical model representing the system, a file format for storing and managing raw files generated from the system and meta-data describing the data contained in the raw files. It supports a variety of data types and is designed for managing huge volumes of data. In order to create HDF5 files the first step is to think about the hierarchy in which the data will be segmented. Then, once the hierarchy has been chosen the raw files can be stored in the corresponding leaf of the hierarchy [22]. This hierarchical data representation allows to create a tree structure that could efficiently segment huge dataset for easy analysis and handling [23]. The benefit of using such format is the ability to efficiently store in an organized manner the data retrieved from the system and also manage the raw files generated.

2. AM data challenges

The specificity of AM processes reside in the nature of the material being created. There is not one specific material that could be relied on during the entire lifecycle of the part. On the contrary throughout the different processes different types of material are created which can be challenging to track and follow the evolution of such materials.

Throughout the AM processes, a lot of different data types and data formats are used and created. This results in challenges when trying to manage and analyze such huge and heterogeneous dataset. The AM product lifecycle is composed of different stages. Each stage encompasses specific types of data and formats that have

been developed in order to answer each AM process's needs [2]. The first stage is the design and focuses on the part model, the recommendation, the topology, the design optimization, the tolerancing, the manufacturability assessment and the material selection. This stage aims to create a digital representation of the part and specify the requirement for the AM processes. The second stage is the process planning and focuses on predicting process response, property and performance response, and process optimization. This stage aims to ensure that the part could be able to be manufactured by preparing the manufacturing plan based on the part design and requirements from the previous stage. The third stage is the build and focuses on anomaly and defect detection, failure detection, machine condition monitoring, real time control, in-situ process monitoring and control. This stage is when the part is actually being manufactured and aims to monitor the manufacturing process. The fourth stage is the post process and focuses on post process control monitoring and control, process end point identification, real time control. This stage aims to prepare and finish the part in order to meet the design requirements. The last stage is the testing and validation and focuses on surface metrology, defect detection and classification. This stage allows the analysis of the resulting part and the comparison against the design requirements.

The heterogeneity of data came from the huge different types of data generated during the AM processes which makes it difficult to efficiently handle, store and analyze. The geometry of the part can be described using different models : the solid geometry, the tessellated geometry, the point cloud geometry, the voxelized geometry. Each of these different types generate specific data formats. The part material can also be characterized using different types of data : the material chemistry, the powder chemistry, the powder microstructure, the powder size distribution, the powder morphology, the powder rheology, the powder thermal properties, the powder optical absorption, the powder optical emissivity. The AM process can be simulated through different angles such as Powder simulation, melt pool simulation, build simulation. The in-situ monitoring generates multiple types of data from : layer wise staring imaging, acoustic monitoring, melt-pool monitoring, layer-wise monitoring. After the machining process, the ex-situ monitoring also generates multiple types of data based on : the microstructure, the X-ray topography.

Thus, there is a need to define a structure that would enable the easy analysis and handling of such datasets and would also take into account the heterogeneity of data types generated throughout the different AM processes.

3. Motivation

AM generates big heterogeneous dataset during its whole product lifecycle making it hard to manage and thus to analyze. The status quo for storing raw files through AM processes is either regular folders, or files format such as Excel. However, in order to apprehend the full potential of AM processes and enhance analytics opportunities, it is crucial to organize and store these big datasets in an effective, usable way. The structures to register, capture and analyze the data are separated and not synchronized which result in time-consuming, labor-intensive data handling and data pre-processing. Moreover, flat structures are used to describe and capture heterogeneous datasets which adds another difficulty for data curation.

Thus, thanks to its hierarchical structure HDF5 could be a key enabler to represent AM data. Hierarchies can be created to store efficiently and comprehensively huge datasets allowing for easy access of AM data and then enhanced analysis. HDF5 also allows for chunking of data, thus based on the hierarchy, the dataset can be separated in different chunks for faster and easier use.

III. Proposed approach for AM hierarchical data organization

1. Description of the approach

Our goal for developing HDF5 data organization for AM is to be able to manage the different datasets generated from the AM processes by coordinating and registering data to facilitate analysis. The structures for

capturing and analyzing will be correlated using a more efficient data management organization. The different data types and formats used during the multiple processes would be reconciled and represented in a unique structure. The data would be compose and compartment, for specific analysis, in order to ensure that only the relevant data is handled for analysis needs.

Our approach will help to organize and store big datasets in an effective way so that raw files are stored in hierarchies making it easy to access and curate. It will support data heterogeneity by enabling the storage of different data types and formats in the same hierarchy. It will facilitate the handling of the data using chunks in order to separate the hierarchies in smaller datasets that are easier to analyze. Finally, it will facilitate data analysis by correlating the data registration structure and the data analysis structure.

2. Hierarchy development

In order to develop a coherent hierarchy, some rules and guidelines must be defined to ensure the validity and usability of the HDF5 file. First, the hierarchies should be developed in a way that all the leaves of the hierarchy should lead to heavy data. Thus, all the buckets containing the data in the leaves of the hierarchies should contain multiple data or datasets. The taxonomy describing the hierarchy should be intuitive in order to facilitate the curation and the chunking of the data. It should ensure that the taxonomy is clear enough to allow for easy identification of the underlying datasets and to prevent any errors of interpretation. The taxonomy should also be deliberate and developed in order to answer AM data challenges. The description of the hierarchy following an analysis purpose will allow to bridge the data registering and the data analysis structure, thus helping the data curation and data processing. The hierarchy should also be agnostic of the process technology. The AM technologies characteristics should not be of importance for the taxonomy development. This will allow to create more generic hierarchies that could be reusable and understandable. Finally, the hierarchy should be developed from a global point of view. It should not be specific to a use case or an application.

Once the taxonomy rules have been identified, the next focus will be on identifying the data to represent. Depending on the AM data challenge's needs, the relevant data should be selected. Then, based on this dataset, different data types and formats, from multiple AM processes, will be involved. Finally, having the datasets and information about the data types and formats, the last step is to think of the composition of the data and how to facilitate the handling of such dataset.

The last step of the hierarchy development is the development of the taxonomy. Once, clear rules for the development and the data have been identified, the taxonomy can be defined. The development of the taxonomy should be driven by context and perspective specific AM data challenges. The focus of the hierarchy should be chosen in order to either develop a goal oriented or generalized hierarchy. Finally, the hierarchy should answer data management needs and help correlate the data analysis and data storage representation of AM data.

3. Hierarchies examples

In order to illustrate our approach, we have worked on four different examples of hierarchies that would allow to answer AM data challenges. The first hierarchy that we are focusing on is the data curation aspect. This hierarchy aims to facilitate the curation of the data by making it easy to store, easy to access and easy to understand. This perspective is important since there are so many different types of format and data produced from and during AM processes. The goal would be for the user to instinctively access and store the data. Thus, the hierarchy needs to be optimized in order that there is no confusion on where to store the data and no confusion on where to retrieve the data. The leaves of the hierarchy should be specific enough so that the type of data in it can be stored only here and nowhere else. However, it doesn't mean that only one type of data can be stored on a specific leaf but multiple data types can be in it as long as they can't be anywhere else.

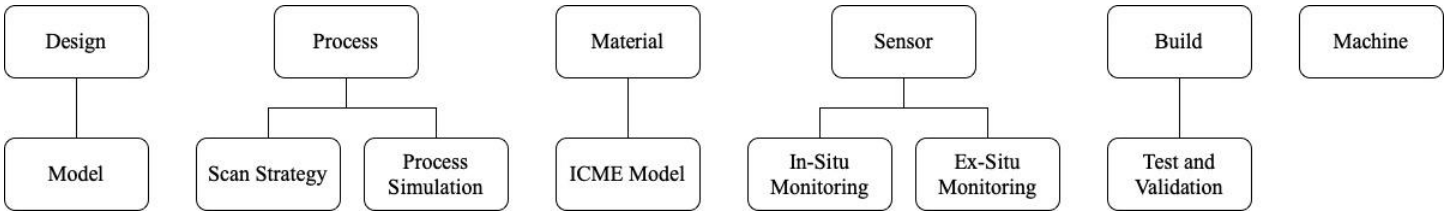


Figure 2 : Data curation hierarchy

This hierarchy aims to describe the AM processes and the data generated in order to create a dictionary of data or a data catalog that could describe and contain all the AM data. The hierarchy is separated into different type of information, design, sensor, build, process, machine, material. Each category contains unique information of the processes or part at this specific point of time during the AM product lifecycle. This hierarchy is a data-centric approach that aims to describe the data in AM processes. However, the hierarchy is not based on data formats, e.g. Image data, Signal data, Geometry data, since it can be difficult to access from an AM perspective and it does not represent AM processes. This hierarchy would allow for easy publication and exchange of the dataset and with a common hierarchy describing the data it would be easier to work in collaboration. The hierarchy would be self-describing allowing for easy use and maintenance by third party. This would also serve as a data catalog to efficiently store the data. This would allow for easy storage and to be a base for the data mining in order to create more advanced data analysis. It would allow for an easy overview of the data available and would ensure that the whole scope of the AM processes could be apprehended.

The second hierarchy focuses on the comparison between the virtual part and the physical part, and on the build replication in production scenarios. The goal is to compare the virtual and physical, observed parts and processes. The main challenge of this hierarchy is to analyze what we are comparing against and what we are validating.

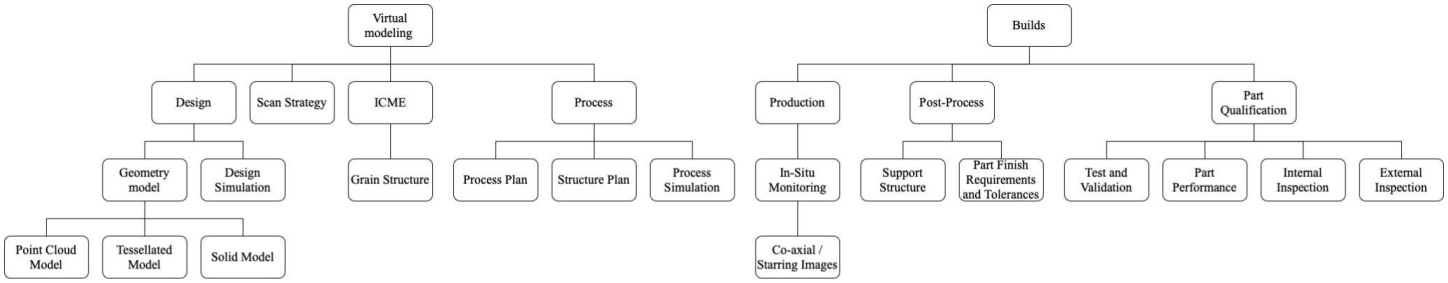


Figure 3 : Part validation hierarchy

The hierarchy of this perspective will create 2 segments containing respectively the virtual part and the physical part. Each side of the hierarchy will focus on the data associated with either the virtual or the physical part. A clear distinction between the 2 parts must be made throughout the processes. Each AM process is analyzed in order to extract the virtual data from the physical data. The data types are not in the center of the hierarchy but each data type is stored in a way that would facilitate the validation of each process. This hierarchy is suited to compare the expected design to the actual part. It allows part validation and comparison against design requirements. Having the data segmented in between expected and measured would allow for easy identification of discrepancies and issues in the resulting part. This hierarchy would also allow for process analysis. Since the requirements for each process are defined, it would be easy to analyze how the process has been made and identify potential errors or optimization capabilities.

The third hierarchy would aim to follow the evolution of the part through the AM Product Lifecycle. The goal would be to track the changes and evolution of the part. e.g. spatial volumes, discrete spaces…, over time.

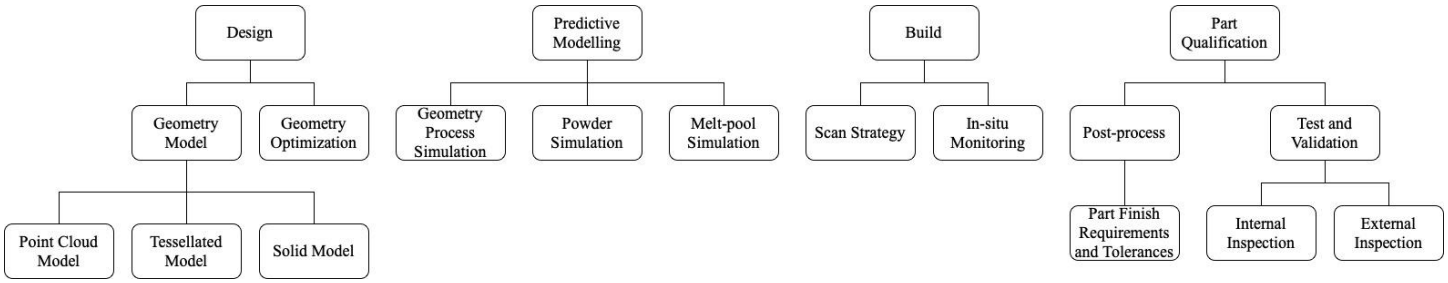


Figure 4 : Product Lifecycle hierarchy

This hierarchy would be separated by each stage of the AM Product Lifecycle. The data generated in each stage would be stored in the corresponding part of the hierarchy allowing to have in the same place the data related to a specific AM process. This hierarchy doesn't aim to capture the "witness specimen" but trace the evolution of the part and what the part looks like at any given time. It is a time-centric approach that captures the state of the part at any given time. It follows as the part matures throughout its lifecycle. This hierarchy would allow the same type of data being stored in different parts of the hierarchy but where the data will be stored depends on which processes the type of data is associated with. This hierarchy would allow to follow the manufacturing of the part and monitor the manufacturing process. Having the hierarchy separated based on the lifecycle stage would allow for users to follow the part even if some part of the processes is externalized. The data from contractors could be stored in the corresponding stage and user could verify the state of the part in its lifecycle. Since each data of the AM product lifecycle is stored based on its stage, this would allow to trace and better control the system. All the data related to the same process will be stored in the same place allowing for easy analysis of a specific process.

This perspective aims to standardize the creation of the material based on the build. The goal is to be suited to be queried by material database. I will develop material information with the design and allow to follow the material evolution throughout the AM processes.

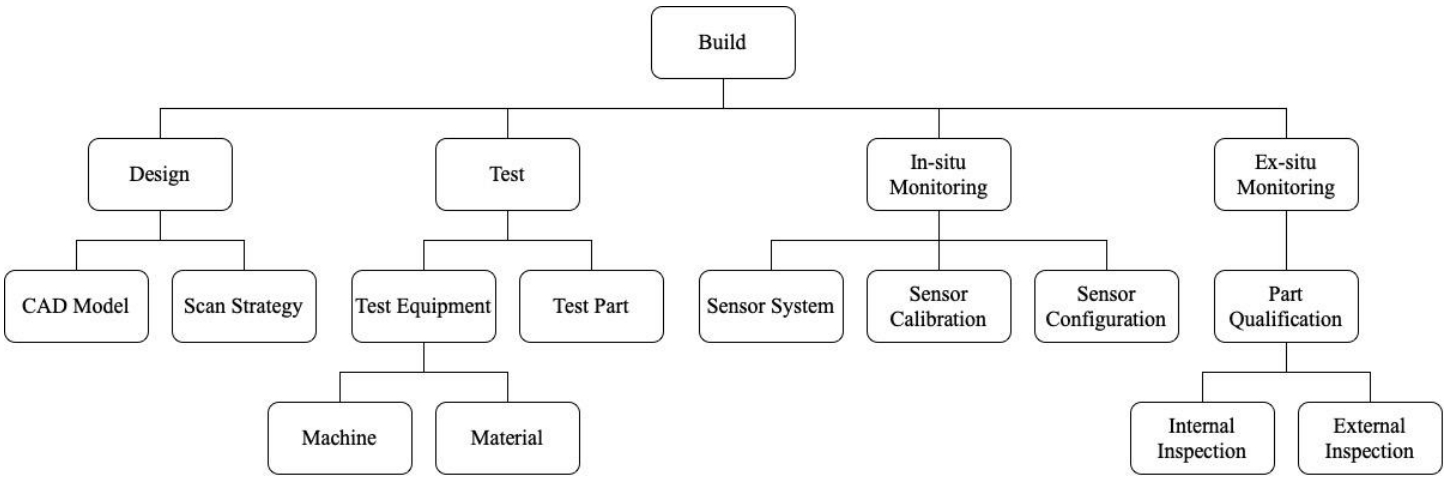


Figure 5 : Material evolution hierarchy

This hierarchy will follow the AMMD model and aims to record and follow the evolution of the material throughout the product lifecycle. The hierarchy will be material-centric and segment the AM processes such as for each part of the hierarchy the material at a specific point of time will be described and the data related to this material will be stored together. The different stages of the material will be segmented and the corresponding processes that allowed the creation of such material will be described in each part.

This hierarchy allows for analysis of the evolution of the material. Thus, this hierarchy would allow for control of the material quality and identification of defects in the material. Having the different stages of the evolution segmented will also allow to identify where the defect might happen and how to improve or modify the process in order to prevent such defect.

IV. Case study applied to Digital Twin

The proposed approach to create a HDF5 hierarchy in order to answer AM data challenges could be applied and used as a basis to build Digital Twin applications. The corresponding hierarchy would contain the information needed to realize the Digital Twin and analysis could be directly realized using the curated and pre-processed data stored in HDF5.

1. Description of the case study

We showcased our approach with a case study obtained from a LPBF build in the Additive Manufacturing Metrology Testbed (AMMT) at NIST [24]. The dataset includes the tessellated geometry of the part, the in-situ monitoring and ex-situ monitoring data. The tessellated geometry contains the 3d representation of the part and the 2d layer-wise geometry. The in-situ monitoring data contains the melt-pool images, the layer-wise melt pool and layer-wise surface. The ex-situ monitoring data contains the XCT images and as-manufactured surface and edges.

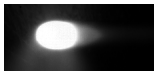
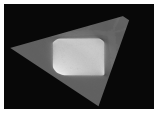
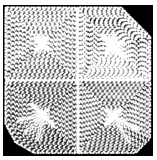
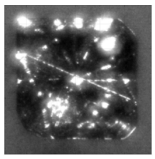
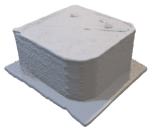
Part geometry	In-situ monitoring	Ex-situ monitoring
 Tessellated geometry	 Melt pool images	 XCT images
 Layer-wise 2d geometry	 Layer-wise melt pool  Layer-wise surface	 As-manufactured surface and edges

Figure 6 : Case study dataset representation [25].

2. Hierarchy for Digital Twin

For this case study, the focus is on analyzing the resulting as-manufactured part and identifying potential defects such as pore structures inside the layer of the part. Thus, the previous proposed hierarchy for part validation (see Figure 3) could be adapted in order to answer the needs to qualify the part. Since the layer-wise geometry and monitoring data will be analyzed, the geometry must be reflected in order to enable easy linking of 2d to 3d data.

Figure 7 represents the part validation hierarchy adapted in order to store the datasets generated by the case study experiment. Each dataset is stored in a leaf of the hierarchy that represents the data contained in the corresponding dataset.

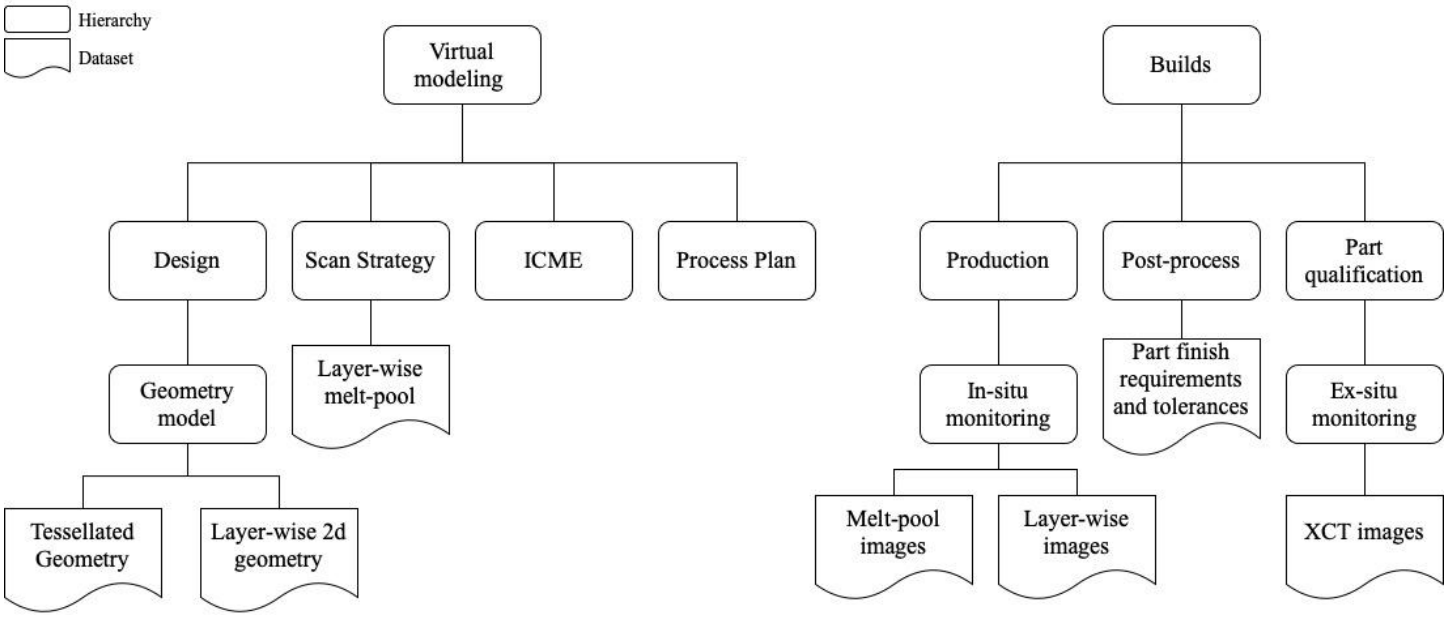


Figure 7 : Case study hierarchy for part validation and Digital Twin development

3. Hierarchy application

Once the dataset has been properly described and stored in the HDF5 hierarchy, multiple applications can be done in order to build replicas and Digital Twins of the part. Since the data is already pre-processed and linked based on layer-wise and geometry data, the analysis on the dataset would be facilitated. For example, using the XCT layer-wise images, Figure 8 shows the 3d XCT volume can be reconstructed which would render data features for the as-manufactured part that could be compared against the tessellated geometry. Defects can be identified inside the different layers of the part and pore structures can be analyzed. The resulting defects that have been found can be compared against the corresponding layer-wise melt-pool and surface to identify potential areas that would lead to such defects. Based on these areas, decisions can be rendered, such as geometry optimization, scan strategy modifications, parameters adjustments…, in order to prevent the observed and identified defects.

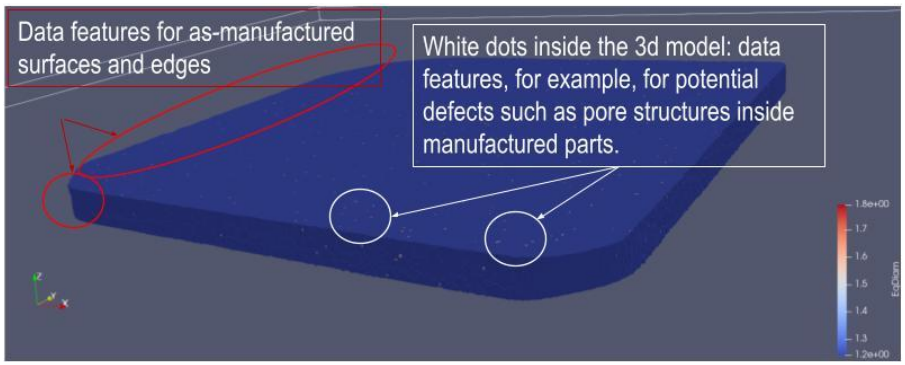


Figure 8 : 3d XCT model reconstructed with defects detection

V. Conclusion

Data generated through AM processes lead to the creation of huge dataset that are heterogeneous in types and formats. Thus, big data management is becoming a growing challenge in AM that impedes the use of the full potential of data analysis. Different methods have been developed in order to help the handling and curation of AM dataset but there is still a lack of common structures between the data registration and the data analysis. In this paper, we have focused on developing a new approach that uses HDF5 in order to store the registered heterogeneous data from different AM processes and allow to directly apply data analysis using the

same structure. We have showcased four different hierarchies that answer specific AM data challenges and would help easy handling and partitioning of big datasets. Finally, we have demonstrated our approach with a Digital Twin application that would allow to use HDF5 as a holder for the data to represent the Digital Twin of the part. Example applications such as defects detection and design optimization can then be easily applied thanks to the coherent hierarchy structure.

In future work, we planned on developing a full data registration structure that would contain larger dataset and showcase the potential of using HDF5 for automated data analysis. The goal will be to focus on the metadata of the datasets in order to describe the data and generate comprehensive pipeline to facilitate data analysis.

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