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A METHOD FOR CHARACTERIZING MODEL FIDELITY IN LASER POWDER BED FUSION ADDITIVE MANUFACTURING

Ibrahim Assouroko*
Université de Technologie de Compiègne
Compiègne, France
Email: ibrahim.assouroko@nist.gov

Felipe Lopez*
University of Texas at Austin
Austin, TX 78712
Email: felipelopez@utexas.edu

Paul Witherell
National Institute of Standards and Technology
Gaithersburg, MD 20899
Email: paul.witherell@nist.gov

ABSTRACT

As Additive Manufacturing (AM) matures as a technology, modeling methods have become increasingly sought after as a means for improving process planning, monitoring and control. For many, modeling offers the potential to complement, and in some cases perhaps ultimately supplant, tedious part qualification processes. Models are tailored for specific applications, focusing on specific predictions of interest. Such predictions are obtained with different degrees of fidelity. Limited knowledge of model fidelity hinders the user's ability to make informed decisions on the selection, use, and reuse of models. A detailed study of the assumptions and approximations adopted in the development of models could be used to identify their predictive capabilities. This could then be used to estimate the level of fidelity to be expected from the models. This paper conceptualizes the modeling process and proposes a method to characterize AM models and ease the identification and communication of their capabilities, as determined by assumptions and approximations. An ontology is leveraged to provide structure to the identified characteristics. The resulting ontological framework enables the sharing of knowledge about indicators of model fidelity, through semantic query and knowledge browsing capabilities.

Keywords: additive manufacturing, model fidelity, model characterization, ontology.

*This work was carried out while the authors were employed as Guest Researchers at the National Institute of Standards and Technology.

1 INTRODUCTION

Additive Manufacturing (AM) processes build objects layer-by-layer directly from three-dimensional models [1]. For years, AM was primarily used to make polymer prototypes. Now, however, AM processes are being employed in the production of end-use parts made of polymers, ceramics, and metals. AM-produced parts are rapidly capturing the attention of the aerospace and biomedical industries who see this technology as suitable for the production of small volumes of highly-complex components [2]. Many issues affect the broader adoption of AM in other industry sectors. Those issues can be traced to challenges with establishing repeatable non-burdening qualification of AM-produced components. Statistics-based quality control techniques, which are often used in the manufacturing industries, are not readily extendable to AM. Extensive testing is required to determine admissible deviations from optimal operating conditions, which are still not well defined in batch-size AM. As an alternative, researchers are trying to move beyond experiments and better incorporate computational models for faster and cheaper part qualification and process optimization in AM [3, 4].

A major challenge in modeling is accounting for and communicating the fidelity of the model. Here, we use the term fidelity as a measure of the extent to which the model faithfully captures and represents its real-world counterpart. Computational models have been developed at different levels of sophistication, resulting in predictions at different levels of fidelity. In the case of AM, for example, there are detailed models that include multiple highly-coupled physical processes, at the expense of requiring many hours of computation time [5–7]. At the other same time, there is an increasing interest in industry for low-cost models that also must make predictions in fractions of a second [8, 9]. Understanding the predictive capabilities of such models requires identifying their characteristics, including their sources of uncertainty.

Good places to start the identification process are the assumptions and approximations that led to the development of the model. The physics of AM processes involve numerous and complex physical phenomena occurring at different length- and time scales. For simplicity, AM processes are often idealized by including only a subset of the phenomena. Even then, a number of simplifying assumptions are usually required to obtain a tractable mathematical model, often in the form of a set of differential equations. These differential equations are further approximated using numerical methods to produce a computational model that can be simulated on a computer. As such, the term assumption is used in the paper to refer to the set of modeling choices adopted by the modeler for the simplification of a physical system, in the course of the development of the mathematical model. Approximation, on the other hand is used to define the set of numerical methods employed to transform the mathematical model into a solvable form.

The development and selection of computational models often involves a balancing act between model fidelity and computational cost. Informed modeling choices should be supported by information on the fidelity of computational models, as determined by their characteristics. Model characteristics are defined as the unique traits of the model, which provide insight into its internal structure and properties. The method proposed in the paper captures such characteristics in an attempt to support the evaluation and communication of model fidelity. This paper builds on a previous study by Witherell *et al.* [10], who proposed an ontology-based characterization of AM models, following their physical domains and the input-output relationships

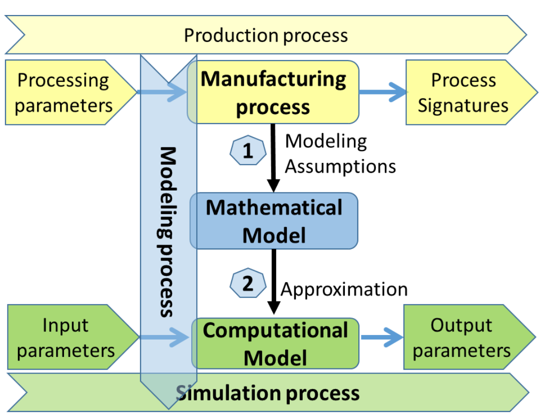

FIGURE 1: The modeling process connecting the worlds of production and simulation processes.

included in their development. We go beyond that classification by incorporating information on modeling assumptions and approximations, to be used as qualitative indicators of model fidelity in laser powder bed fusion (L-PBF) models. Specifically, the ontology provides a formal explicit representation of:

(a) modeling characteristics and their influence in model predictions,
(b) sets of axioms and mathematical rules that define and relate such modeling characteristics.

Qualitative knowledge on model fidelity can be extracted and shared to support informed assessment of L-PBF models.

The remainder of the paper is organized as follows. Section 2 presents the background for structuring and representing information in computational models, and gives insight into the approach proposed for model characterization and representation. Section 3 discusses details of the proposed conceptualization and characterization of L-PBF models. Section 4 presents the main elements of the resulting ontological framework, and discusses the support it provides in the identification and exchange of qualitative indicators of model fidelity. Finally, Section 5 presents some conclusive remarks, including the description of future work with focus on 1) the extension and validation of the proposed framework and 2) quantitative assessment of the influence of the identified modeling characteristics in model fidelity.

2 BACKGROUND

Some approaches have been proposed previously for the study of the information incorporated in computational models [11–13]. For instance, Bryden and Noble [11] discussed the requirements for the description of models and proposed a framework to describe the process of scientific modeling, which is similar to the one illustrated in Figure 1. Alternatively, Bedau [13] discussed the notion of “unrealistic” models and provided practical means to quantify potential discrepancies between models and the real world. Along similar lines, Di Paolo *et al.* [12] discussed 1) the need for a proper understanding of the internal operations of computational models and proposed 2) a methodology to reconcile potential discrepancies between computational models and experiments. Such a methodology would allow the modeler to determine where differences between models and the real world lie, and to assess the usefulness of such models.

The work of Di Paolo *et al.* suggests that a clear understanding of the internal operations of computational models could potentially help quantify levels of fidelity. As a result, methods that support clear and explicit representations of the internal operations of models are increasingly sought after as a means to determine the influence of those operations on model inadequacy. Such an explicit representation could be used to return qualitative indicators of the degree of model fidelity. Those indicators could be stored for future use in a knowledge-based system.

Knowledge-based systems have been proposed in various domains to support design and analysis in engineering [14, 15]. Other types of knowledge-based frameworks have been proposed to represent physical systems at various levels of abstraction [16, 17]. Similar knowledge-based frameworks have been proposed across other engineering domains [18–21]. Ontologies provide popular foundation for creating many of these knowledge-based systems. Ontologies have been used to provide definitions of formal methods in modeling, while also addressing aspects of model fidelity [22–24]. In this paper we aim to use ontologies to represent the variety of information needed while addressing fidelity-related issues in computational models of L-PBF processes.

Fidelity problems in L-PBF models can originate from multiple sources, including certain internal characteristics of the model itself. In this article, we identify and map those sources to specific modeling elements, based on the assumptions and approximations adopted in the modeling process. Certain questions that help with these problems have been identified, and they are:

(a) what are the most appropriate mathematical models to represent a physical phenomenon?;
(b) what set of assumptions would be required to accurately define a given L-PBF model?;
(c) which physical law, initial and/or boundary conditions, material properties, etc. are usually employed in the definition of a given mathematical model?;
(d) which modeling characteristics are most likely to affect the fidelity of a given model in L-PBF?;
(e) how do these fidelity-related characteristics interoperate with other influential modeling elements?.

Answering these questions can help us identify the requirements and scope of L-PBF model abstractions. In creating such abstractions, we plan to use a descriptive ontology to form the basis of a knowledge-based framework. The ontology can be used to 1) browse and represent the sets of model characteristics available for the definition of a given L-PBF model and 2) provide insight into potential qualitative indicators of model fidelity. The framework can help classify the requirements for both model characteristics and model usages.

3 CHARACTERIZING PREDICTIVE CAPABILITIES OF POWDER BED FUSION MODELS

Assessment of the fidelity of an AM model unavoidably depends on the particular case being simulated (i.e., material properties, machine information, and process parameters), the adopted simulation parameters and the predictions of interest. Quantitative evaluation of model fidelity is possible with uncertainty quantification, which measures the individual contribution of various sources of uncertainty and their influence in the overall prediction uncertainty [25]. Without being specific to a particular case, the characteristics of such models can also be used to drive qualitative estimates of fidelity. In other words, knowing what capabilities a model has and lacks allows users to estimate how accurate model predictions may be if the right simulation inputs are provided.

Model characteristics in AM, as defined by assumptions and approximations, are determined during the modeling process (illustrated in Figure 1). Therefore, abstracting some common assumptions and approximations taken when modeling AM processes can help identify some of those characteristics. Examples of model characteristics can be found in the physical domain, physical laws, boundary and initial conditions, and the chosen numerical method, among others.

Model characterization can be performed for various types of models. For different types of models, the characterization methods may be similar, but the underlying physics and model form would differ. The phenomena presented in this paper are limited to irradiation absorption, heat transfer, and consolidation in L-PBF processes. In this section, the physics of each phenomenon and available model types are identified along with common modeling assumptions and approximation. Information on model characteristics is organized in the form of tables to aid visualization and facilitate their definition in the ontology introduced in section 4.

3.1 Irradiation absorption models

Irradiation absorption is related to how voids in a randomly-packed bed allow the laser beam to penetrate and reflect from the surface of powder particles. Computational models of irradiation absorption have been developed to predict the amount and distribution of the heat that is absorbed by the bed. Table 1 shows some common choices, found in the literature, for such models, including their characteristics as identified from assumptions and approximations. As seen in the table, each model depends on a governing physical law, which in turn depends on a combination of the following assumptions made by the modeler:

(a) Whether heat is assumed to penetrate the powder bed and adopt a volumetric distribution in the model or to be constrained on the surface.
(b) If the powder bed is idealized as a continuum or modeled as a distribution of interacting powder particles.

Common combinations of assumptions and the physical law of choice for such cases are presented in Table 1, along with numerical solution methods. For instance, in the simplest case, where absorption is assumed to be restricted to the surface, no mathematical model is required. This scenario can be found in the first line of the table. Other choices for absorption models (i.e., Beer-Lambert model, ray tracing models, or radiation transfer models) are available when absorbed energy is assumed to have a volumetric distribution. The type of distribution assumed for

Dimensionality of absorbed energy	Distribution of material	Surface distribution of heat source	Law of Physics	Mathematical model	Numerical method	Model inputs	Output parameters	Ref.
Surface	Continuum	Gaussian, cylindrical, or point source	Beer-Lambert law	Beer-Lambert model		Absorptivity and surface irradiation	Surface distribution of absorbed heat	[26–31]
Volumetric	Continuum	Gaussian, cylindrical, or point source				Absorptivity, extinction coefficient, surface irradiation	Volumetric distribution of absorbed heat	[32, 33]
Volumetric	Particles	Gaussian	Specular reflection	Ray tracing model	Discrete element method	Surface irradiation, particle size and distribution, dimensions of powder bed, latent heat, absorptivity, and emissivity and reflectivity of particles	Volumetric distribution of absorbed heat	[34–36]
Volumetric	Particles	Gaussian	Radiation transfer	Radiation transfer model	Two-flux method	Surface irradiation, particle size, specular reflectivity, thermal conductivity, and melting temperature	Volumetric distribution of absorbed heat	[37–40]

TABLE 1: Modeling characteristics for irradiation absorption models.

the laser, which strongly influences the quality of the predictions, is shown as another characteristic of irradiation absorption models. Such information can guide experienced users to identify the amount of fidelity to be expected from each case. Additionally, the adoption of a larger set of input parameters increases the flexibility of the model, allowing it to adapt to more cases and increasing the fidelity that might be expected from it.

The fidelity to be expected from irradiation absorption models is strongly dependent on how close the simulation model is to the physical events it is meant to describe. For example, the Beer-Lambert law, which assumes an exponential decay for irradiation intensity as a function of depth, imposes a constraint on the simulation model that reduces fidelity. In the ray-tracing models, on the other hand, laser rays are assumed to bounce from powder surfaces based on the size and distribution of the powders. This bouncing seems to capture reality very well. As a result, a ray-tracing model, which does include laser-particle interactions, provides higher fidelity predictions than a Beer-Lambert model. Similar fidelity issues appear with simulation inputs that are accounted for or neglected (more inputs increase flexibility of the model and potentially improve its fidelity), the choice of numerical model, and other model characteristics.

3.2 Heat transfer models

Heat absorbed from the laser is dissipated through the powder bed, heating and consolidating the powder. Heat-transfer models attempt to predict 1) the distribution of the solid, liquid and mushy zones in the powder bed as well as 2) the temperature distribution in each zone. Given the complexity of the heat transfer phenomenon, which includes a large set of model characteristics, the modeler has to go through a series of modeling choices and simplification steps to fully determine whether thermal models are ready for simulation. The characteristics identified on models in the literature, as imposed by their underlying assumptions and approximations, are presented in Table 2.

At the macroscale level, all models are based on two laws: Fourier's law and conservation-of-energy law. The resulting mathematical model takes the form of a transport, partial-differential equation (PDE) for a chosen combination of transport property (thermal diffusivity or thermal conductivity) and a state variable (temperature or enthalpy). There is little difference in the fidelities of any of these combinations; but, it is still important for the user to know which combination has been adopted to determine the type of heat equation to be solved. For simplicity, the PDE is shown here for temperature as the state variable and thermal conductivity as the transport property[1]

$$\rho c_p \left(\underbrace{\frac{\partial T}{\partial t}}_{\text{time}} + \underbrace{\vec{v} \cdot \nabla T}_{\text{advection}} \right) = \underbrace{\nabla \cdot (k \nabla T)}_{\text{diffusion}} + \underbrace{f(x,y,z)}_{\text{source}}, \qquad (1)$$

where powder density is denoted by ρ, specific heat is c_p, thermal conductivity is k, volumetric heat generation is f, and $\vec{v}$ is the velocity in the fluid phase. In this equation, the advection term is often ignored if fluid flow is neglected[2]. It should also be noted that absorbed heat, as computed with the irradiation absorption model, can be accounted for either as a source or as a boundary condition (if assumed as a surface source).

[1] The structure of the heat transfer equation for other choices of state variable and transport property is similar. For a detailed discussion, refer to the classical book of Carslaw and Jaeger [45].

[2] The scope of this paper includes only models with no fluid flow.

Law of Physics	Transport property	State variable	Reference frame	Dimensionality of absorbed heat	Inclusion of absorbed heat	Phase change	Mathematical model	Model inputs	Boundary conditions	Initial conditions	Distribution of material	Numerical method	Prediction	Ref.
Conservation of energy and Fourier's law	Thermal conductivity	Temperature	Moving or fixed	Surface or volumetric	Source term	Implicit (included in specific heat) or explicit	Transport equation for temperature	Powder density, specific heat, fluid velocity, absorbed heat	Semi-infinite, adiabatic, isothermal, or mixed	Initial distribution of temperature	Continuum	Finite element method, finite difference method	Time-history of temperature	[41]
Conservation of energy and Fourier's law	Thermal conductivity	Temperature	Moving or fixed	Surface or volumetric	Source term	Implicit (included in specific heat) or explicit	Transport equation for temperature	Powder density, specific heat, fluid velocity, absorbed heat	Semi-infinite, adiabatic, isothermal, or mixed	Initial distribution of temperature	Particles	Discrete element method, Lattice Boltzmann method	Time-history of temperature	
Conservation of energy and Fourier's law	Thermal conductivity	Enthalpy	Moving or fixed	Surface or volumetric	Source term	Implicit (included in specific heat) or explicit	Transport equation for enthalpy	Powder density, specific heat, fluid velocity, absorbed heat	Semi-infinite, adiabatic, isothermal, or mixed	Initial distribution of enthalpy	Continuum	Finite element method, finite difference method	Time-history of enthalpy	[27,28, 30,42]
Conservation of energy and Fourier's law	Thermal conductivity	Enthalpy	Moving or fixed	Surface or volumetric	Source term	Implicit (included in specific heat) or explicit	Transport equation for enthalpy	Powder density, specific heat, fluid velocity, absorbed heat	Semi-infinite, adiabatic, isothermal, or mixed	Initial distribution of enthalpy	Particles	Discrete element method, Lattice Boltzmann method	Time-history of enthalpy	[43,44]
Conservation of energy and Fourier's law	Thermal diffusivity	Temperature	Moving or fixed	Surface or volumetric	Boundary condition	Implicit (included in specific heat) or explicit	Rosenthal-type equation	Powder density, specific heat, fluid velocity, absorbed heat	Semi-infinite	Initial distribution of temperature	Continuum	Analytical	Time-history of temperature	[31]

TABLE 2: Modeling characteristics for heat transfer models.

The terms included in the heat transfer equation can be used as indicators of the predictions that may be obtained from solving the model. For instance, transient thermal predictions (i.e., thermal history) may only be obtained if the time derivative is included in the equation. Additionally, the effect of melt pool dynamics in the thermal history can only be accounted for if the advection term is present in the heat transfer equation and it takes velocity predictions from a fluid mechanics model. The lack of any of these terms compromises the fidelity of the thermal predictions obtained from the model.

The mathematical problem is completed with adequate choices of models for phase change, and a set of boundary conditions. In the case of transient simulations, initial conditions are usually required as the starting point. Phase transformations may be ignored, modeled explicitly with a Stefan condition, or included in the form of a temperature-dependent specific heat. Most models use as boundary conditions a mix of convection, radiation and surface distribution of heat atop the powder bed; adiabatic boundary conditions on the side while the bottom is often semi-infinite, adiabatic, or in contact with a substrate.

If one assumes constant thermo-physical properties, neglects phase changes, and uses a reference frame attached to the heat source, a special type of thermal model can be created. This model is special because an analytical solution can be obtained for the temperature distribution as a function of thermal diffusivity [31]. Although simplistic, Rosenthal-type models provide 1) starting points in the development of more sophisticated models and 2) quick predictions of temperature and melt-pool geometry.

In general, simpler models, such as Rosenthal models, typically return predictions with less fidelity than more elaborate models such as lattice Boltzmann models and discrete-element models. Additionally, the adoption of a continuum to represent a bed of particles is expected to compromise the fidelity of the predictions making them similar to those reported in irradiation absorption models. Finally, the choice of boundary conditions is one of the most important characteristics that guide the user in

Material	Law of Physics	Consolidation mechanism	State variable	Mathematical model	Initial condition	Model inputs	Prediction	Ref.
Amorphous or crystalline	Atomic diffusion in crystal vacancies	Solid state sintering	Volume	Frenkel	Initial volume	Surface tension, diffusion coefficient, temperature, Boltzmann's constant, crystal lattice constant	Volume	[46]
Amorphous	Newtonian flow	Solid state sintering	Density or porosity	Mackenzie and Shutthelworth	Initial powder density	Surface tension, number of pores per unit volume, material viscosity	Density or porosity distribution	[47]
Crystalline	Non-Newtonian flow	Solid state sintering	Density or porosity	Mackenzie and Shutthelworth	Initial powder density	Surface tension, number of pores per unit volume, material viscosity, tuning parameter	Density or porosity distribution	[47]
Crystalline	Temperature-activated reaction	Solid state sintering	Density	Arrhenius-type equation	Initial powder density	Characteristic frequency, sintering activation energy, ideal gas constant, temperature, tuning coefficients	Density distribution	[48]
Crystalline or semi-crystalline	Temperature-dependent density	Melting	Density or porosity			Temperature, melting temperature	Temperature-dependent powder density	[27]

TABLE 3: Modeling characteristics for consolidation models.

the level of fidelity to be expected from heat transfer models. The incorporation of more accurate boundary conditions is expected to greatly improve the fidelity of a model.

3.3 Consolidation models

Thermally-activated consolidation is responsible for transforming selected regions of powdered material into fully-dense parts. Consolidation is of crucial importance in AM because most mechanical properties (e.g., tensile strength) have been found to decrease drastically whenever the porosity increases. In PBF processes, consolidation may occur by 1) solid state sintering, controlled by viscous diffusion; 2) partial melting, where part of the powder is melted while the rest remains solid; and 3) full melting, characterized by the rapid melting of all the heated powder into fully-dense material [49]. The physics of these mechanisms are substantially different and depend on the choice of material to be processed meaning that not all materials can be sintered or melted.

Table 3 provides information on the characteristics and modeling choices available for the definition of a consolidation model, which differ depending on whether the material is crystalline (ceramics, metal alloys, hard metals) or amorphous (amorphous and semi-crystalline thermoplastics).

In the case of sintering, a model is required to describe the variation in density as a function of temperature and time. A mathematical model, in this case, must be based on only one of these four physics principles: atomic diffusion in crystalline vacancies for Frenkels model [46], Newtonian or non-Newtonian flow for Mackenzie and Sutthelworths model [47], temperature-activated reaction for an Arrhenius-type equation [48]. Melting, on the other hand, is much faster and it is often assumed that density varies instantaneously when reaching melting conditions, thus not requiring any specific mathematical model.

For sintering, consolidation models are often governed by ordinary differential equations. For melting, consolidation models are governed by temperature-dependent properties. Both have simpler mathematical forms than heat transfer models. The definition of well-defined consolidation models requires only initial conditions (initial density), and coupling to thermal models that determine the numerical approach used to solve the system (numerical method, grid, solver, etc.).

The choices available in consolidation models are not driven by their expected fidelity. Rather, they are driven by the physical laws that govern the consolidation mechanism. Consequently, an incorrect choice of physical law could compromise the fidelity of the predictive model significantly. For example, using the physical laws governing solid state sintering when developing a model of the process used to fully melt metallic powder.

Tables 1 to 3, show that the prediction outputs of some models can be used as inputs to other models. As a result, more elaborate predictions can be built up from 1) the predictions obtained from simpler models and 2) a set of relationships that capture their inter-operation. For example, consolidation models determine density, which is an input in thermal models, which in turn determine temperature, which drives consolidation. Such rules are included in the ontology, to guide users along the modeling process and provide explicit knowledge about how model characteristics influence predictions that could be returned by models of other types.

4 AN ONTOLOGY TO LEVERAGE THE CHARACTERIZATION

We turn to OWL 2 Web Ontology Language [50] to formalize our proposed characteristics into an ontology and its associated knowledge-based framework that provides more means for reusability. The ontology was implemented using Protégé [51], a Java-based ontology development software tool developed by Stanford University. The ontological concepts described in this paper extend those discussed in [10]. Here we extend the categorical representation of those concepts by adding specific attributes to support the characterization of model fidelity. This enhanced ontology provides an explicit description of all the new concepts and their relationships. It connects the physics with the corresponding modeling concepts. In addition, the ontology should capture knowledge about the assumptions used in creating mathematical models, in choosing their input parameters, and in finding the solutions. The information in this ontology can be used to extract and navigate explicit knowledge about the specific characteristics affecting the fidelity of a given L-PBF process model. This knowledge then could serve as indicators to enhance the user's ability to 1) estimate the expected level of fidelity, and 2) make informed decision about the models reusability.

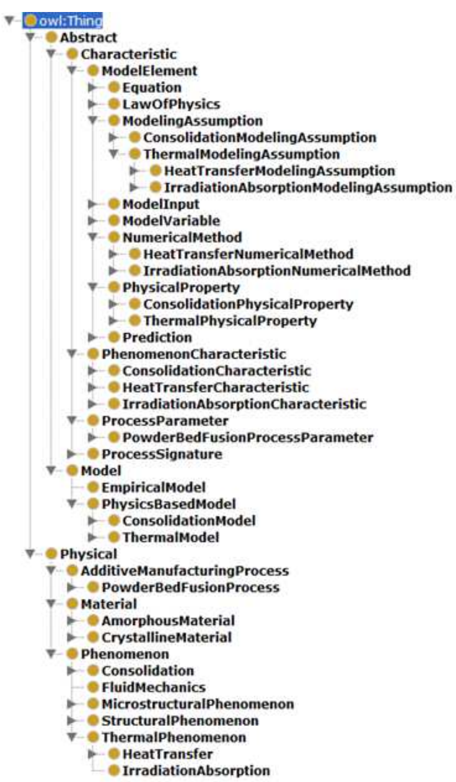

FIGURE 2: Taxonomy of top level entities in the AM ontology.

4.1 Hierarchy of the ontology

Figure 2 illustrates the hierarchical structure of most important high level entities in the AM ontology. This ontology is structured as two main AM concepts:

(a) the **Physical** concept that includes everything that has a position in the space-time domain and;
(b) the **Abstract** concept that includes everything else.

In essence, the separation between real and simulated is made at the highest level at the ontology.

Under **Physical**, we have the concepts of **AdditiveManufacturingProcess**, **Phenomenon**[3] and **Material**. **Phenomenon** is understood as an observable event, including input and output flows of matter and energy, which cannot be divided in smaller phenomena. **Material** briefly covers the different types of material families used in AM. **AdditiveManufacturingProcess** and **Phenomenon** are described as two different **Physical** entities; but, they are not completely disjoint, since a phenomenon (or a set of phenomena) can only occur during the course of a process.

Abstract entities are organized into two main concepts: **Model** and **Characteristic**. The notion of **Characteristic** is central to this ontology. There are two kinds of characteristics. The first are modeling characteristics, as defined in Section 3. The second are physical characteristics, which have a number of sources including machine vendors, material vendors, process engineers, and the dynamics of the process itself. Details of the modeling characteristics are presented in Tables 1 to 3.

The concept of **Model** is understood as a mathematical object that has the ability to represent a system or one of its components and to predict behavior of either. The mathematical object is valid for a set of defined conditions and simplified assumptions [52], which are likely to affect the fidelity of the model. A **Model** can be physics-based, empirical, or hybrid. In this paper, we focus only on physics-based models. A **PhysicsBasedModel** is referred to as a mathematical (or computational) model that describes some physical phenomenon based on first-principles and physical laws. Examples of physics-based model are:

(a) **HeatTransferModel** based on Fourier's law and energy conservation law, as characterized in Table 2;
(b) **IrradiationAbsorptionModel** based on, either Beer-Lambert law, radiation transfer law or physical reflection law, as provided by Table 1 and;
(c) **ConsolidationBySinteringModel** describing a Newtonian or non-Newtonian flow, or a temperature-activated reaction for a given material, under a certain processing conditions, as described in Table 3.

The concept of **Characteristic** subsumes four different types of abstract entities: **ModelElement**, **PhenomenonChar-**

[3] Although often similar to a phenomenon, in this article, the term "process" is reserved only for manufacturing processes and does not include the occurring phenomena pertaining to those processes.

acteristic, **ProcessParameter**, and **ProcessSignature**. **ModelElement** as proposed in the actual study, includes **ModelingAssumption**, **Equation**, **PhysicalProperty**, **ModelInput**, **ModelVariable**, **NumericalMethod** and **Prediction**. These entities are used, along with the modeling process, illustrated in Figure 1, to characterize a physics-based model. They can be assigned and coupled based on the step(s) in which they appear. These entities are important because they can impact model fidelity negatively. Such negative impacts result from the discrepancies introduced along the transition from a physical phenomenon to the mathematical model that represents it. These discrepancies can impact predictions obtained from solving the model.

A first level of discrepancy might involve an incorrect **ModelingAssumption**. For example, an incorrect physical law might be chosen to capture a simplification of a physical system, and the resulting predictions will be farther from what is believed to happen in reality. Another type of discrepancy can occur if the appropriate set of **Equation** entities are not chosen to describe a mathematical model. In this case, the predictions from the associated computational models will have less fidelity. Fidelity can also be lost or improved depending on whether the right set of **PhysicalProperty** and/or **ModelInput** entities are assigned for the simulation of a computational model.

In assessing fidelity-related issues, the preceding fidelity indicators are not enough. Consequently, the ontology should provide explicit, descriptive knowledge of these indicators sufficient to do a quantitative assessment of the predictive capabilities of the model in which they appear. This knowledge is provided in two forms, which are: knowledge about the defined AM modeling concepts and knowledge about the relationships among those concepts. These relationships are discussed in the following sections.

4.2 Taxonomy of relationships in the ontology

Relationships in the ontology have been created to define interconnections between any physical, abstract entity and its parent and child. Physical concepts, such as **Phenomenon**, interrelate with abstract concepts, e.g., **PhenomenonCharacteristic** through the role *hasCharacteristic*, and physics-based models interrelate the phenomenon(a) they describe through the role *represent*. The *partOf* relationship has been defined to accommodate the fact that two different concepts can exist at the same level of hierarchy with one still being part of the other, instead of defining a parent-child relationship between them. Example of this specificity in the current ontology is between **AdditiveManufacturingProcess** and **Phenomenon** where a phenomenon is not a subclass of an AM process but can only occur within the course of that process. The concept of **Characteristic** is defined along with the role *influences* (as inverse of *influencedBy*) that can exist between a characteristic, e.g. **HeatDissipationCharacteristic**, and one or several physical concepts, e.g., **Consolidation** and **FluidMechanics**. Some **ModelElement** concepts are semantically related to other abstract concepts they characterize (or are characterized by) through several relationships such as *definedBy*, *requires* and related sub-properties (*requiresAssumption*, *requiresInput*, *requiresApproximation*), *provides*, etc.

Illustrations of such interconnections are shown on Figure 3 to Figure 5, where several object properties are used to interrelate the different concepts playing roles in the characterization of irradiation absorption model, heat transfer for temperature model, and consolidation model.

4.3 Semantic queries allowed by the ontology

Ontologies support different levels of queries using query language such as SPARQL [53], and query tools such as SPARQL Query and DL Query tabs in Protégé [51]. At a first level are simple queries that can provide answers to a range of competency questions. Two examples of such queries (using DL Query tab) are given below:

(a) In the first example related to sintering model, the ontology is queried for the current equation used to predict density variations for crystalline materials in AM. The query returns ArrheniusTypeDensityVariation and CrystallineDensityVariation equations, which are the appropriate choices for that question.
(b) In the second example, one may be interested in knowing 1) which modeling parameter is influenced by variations in specific heat and 2) which phenomena this parameter influences the most. The query returns thermal diffusivity as the parameter; and heat transfer, consolidation and fluid mechanics as the phenomena.

More complex queries can be executed, as well. Typically, such queries attempt to retrieve information on the specific characteristics that determine and influence the quality of the predictions provided by a physics-based model, and their interconnections throughout the modeling transition, described in Figure 1. Figure 6 shows the possible transitions for the modeling and computation of a distribution of absorbed heat. These transitions result from the combination of complex sets of DL-queries on indicators and influencing characteristics including the nature of the heat source and the distribution of material, among others. Using this modeling transition graph, users can then retrieve additional knowledge about other specific concepts likely to affect the fidelity of the absorption model.

5 CONCLUSIVE REMARKS

Computational models in AM often face reusability challenges, partially driven by the limited understanding of a model's fidelity and the lack of knowledge that users have on the com-

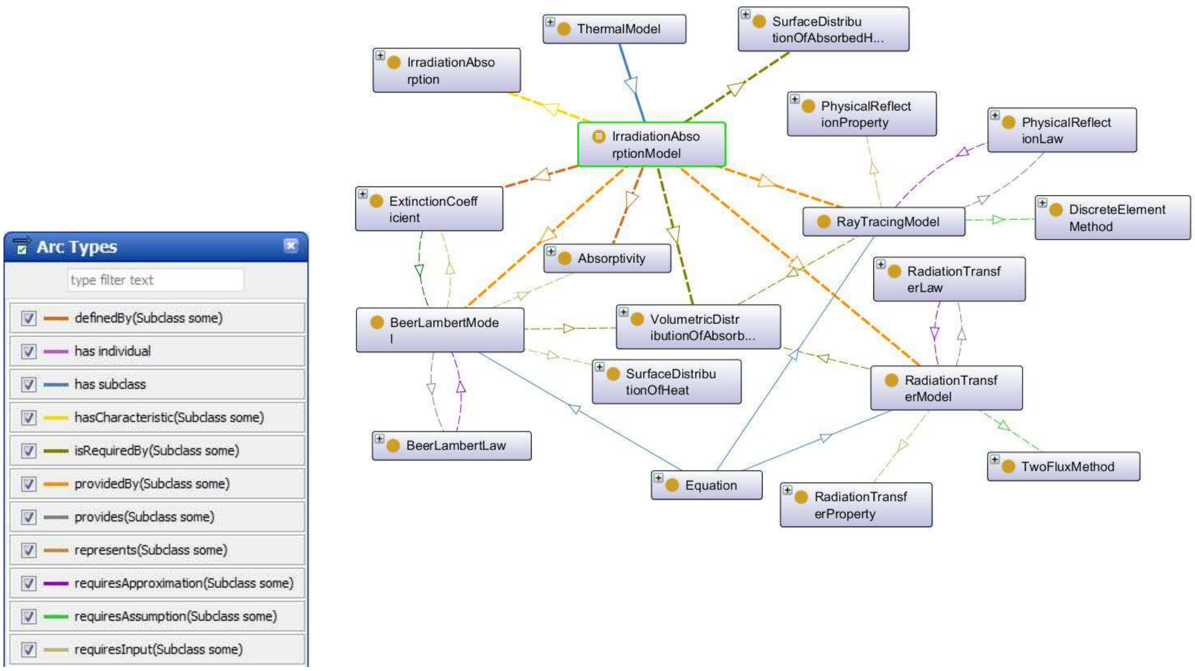

FIGURE 3: Relationships of irradiation absorption model.

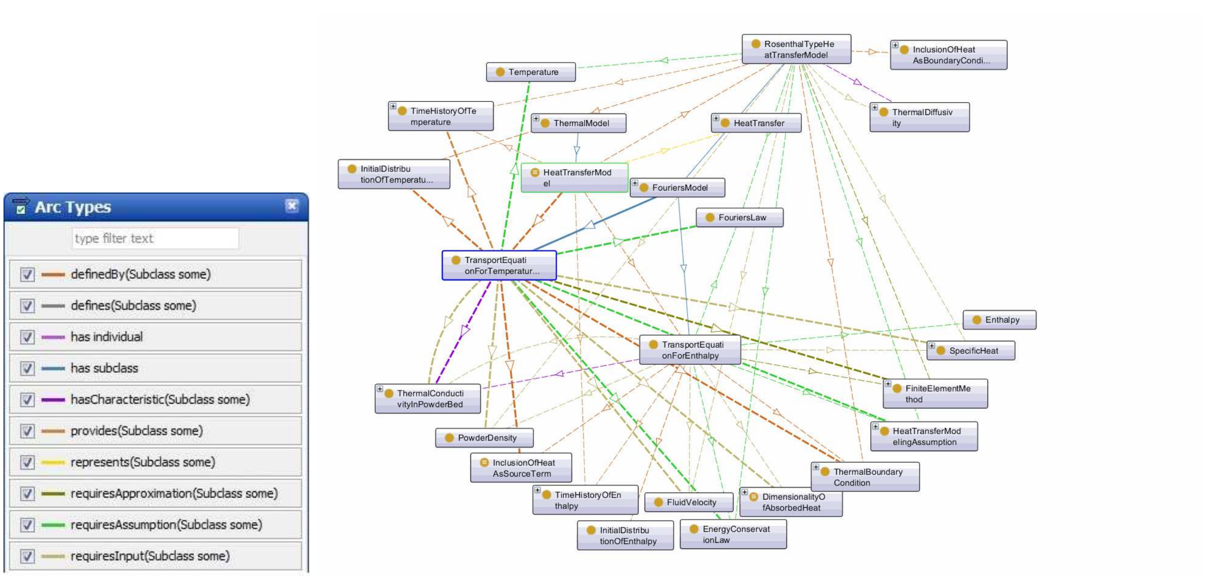

FIGURE 4: Relationships of heat transfer model.

petences and performance of the models. To better understand the unique characteristics that determine predictive capabilities of the models, a closer look has been given to the abstractions formed between physical processes and corresponding computational models.

This study sought a better understanding of the limitations in the predictive capabilities of physics-based models in AM. Our approach to achieve that understanding was based on explicit characterizations of the assumptions and approximations used to develop the corresponding computational models. We expressed these characterizations as sets of formal concepts in an ontology. The ontology provides the information needed to answer a wide

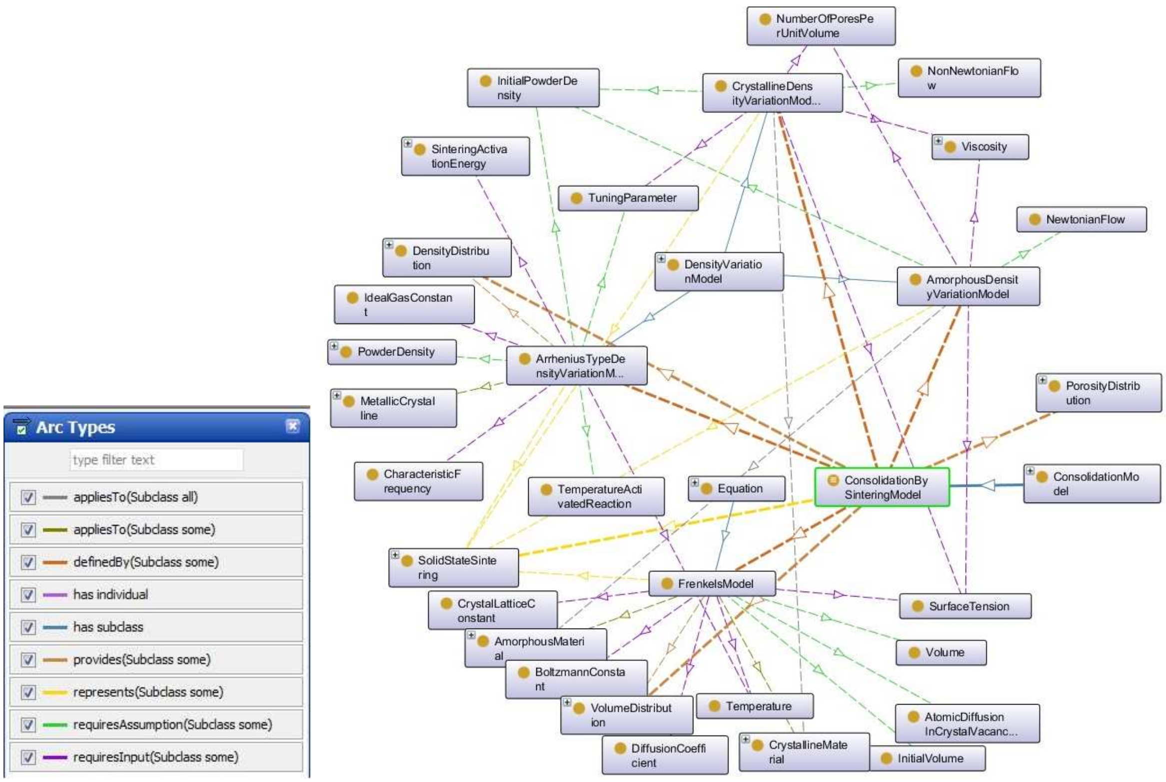

FIGURE 5: Relationships of consolidation model.

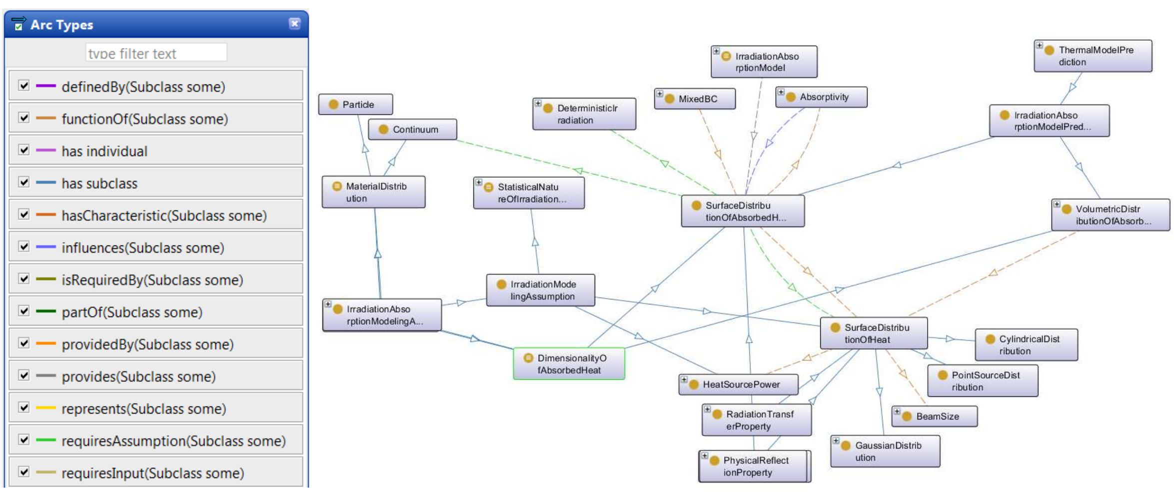

FIGURE 6: Modeling transition for absorbed heat.

range of competency-related and fidelity-related queries. Those queries are currently based on thermal and consolidation models only.

We intend to expand the ontology to address the impacts of assumptions and approximations on the predictive capabilities of fluid mechanics models, structural models, and microstructural models. Another ongoing work at NIST focuses on the origin and propagation of uncertainty sources in additive manufacturing models [25] and is expected to be incorporated into this work in future implementations.

SUPPLEMENTAL MATERIAL

The ontology described in this paper can be accessed at https://github.com/usnistgov/AMontology

DISCLAIMER

The full descriptions of the procedures used in this paper may require the identification of certain commercial products. The inclusion of such information should in no way be construed as indicating that such products are endorsed by NIST or are recommended by NIST or that they are necessarily the best materials, instruments, software or suppliers for described purposes.

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