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ONTOLOGY-BASED LASER AND THERMAL METAMODELS FOR METAL-BASED ADDITIVE MANUFACTURING

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ABSTRACT

Additive manufacturing (AM) is a promising technology that is expected to revolutionize industry by allowing the production of almost any shape directly from a 3D model. In metal-based AM, numerous process parameters are highly interconnected, and their interconnections are not yet understood. Understanding this interconnectivity is the first step in building process control models that help make the process more repeatable and reliable. Metamodels can be used to conceptualize models of complex AM processes and capture diverse parameters to provide a graphical view using common terminology and modeling protocols. In this paper we consider different process models (laser and thermal) for metal-based AM and develop an AM Process Ontology from first-principles. We discuss and demonstrate its implementation in Protégé.

Keywords: additive manufacturing, ontology, thermal model

1. INTRODUCTION

Additive Manufacturing (AM) has seen considerable growth in the past five years. According to the Wohler's Report, in 2013 the compounded annual growth rate over 25 years was 25.4 % while the compounded growth rate was 27.4 % from 2010 to 2012 (\$2.2 billion) [1]. The development of AM is driven by industries seeking to produce parts with complex geometries, as is often required in aerospace, automotive, and biomedical applications [2]. However, there are still many challenges for the AM industry, such as the lack of a wide variety of materials, poor part accuracy, residual stresses, low repeatability, and the lack of methods for qualification and certification [2, 3]. Moreover, the lack of understanding of the complexity and mechanisms involved in the actual AM processes create challenges in predicting residual stress [4, 5], mechanical properties caused by porosity and distortion due to heating [6]. Microstructures generally depend on the thermal history of the heat source and have a strong influence in the mechanical properties of the 3D printed parts [7, 8]. While these correlations are under study, variations in AM processing parameters, processing environments, and measurements create situations where results (e.g., models, data, etc.) are difficult to compare and contrast. Furthermore, homogenization and aggregation of data sets is needed to establish the correlations that can provide insight into microstructural evolution, for example, from the thermal history of the build to mechanical properties of the finished part. Metamodels are able to help us homogenize model-driven data sets, and thus generalize correlations, which in turn will help in ensuring process repeatability and reliability.





Figure 1 shows a schematic of important elements in AM from an integrated viewpoint, as introduced by Huang *et al.* [2]. Materials development and evaluation is a requirement for predicting material properties and broadening the scope of applicability of AM. Design methodologies can improve freedom and create opportunities for customization with better functionality. Modeling, monitoring, and control of processes are critical to achieving AM process stability. Characterization and

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certification are necessary to enhance repeatability and quality of the manufactured product. These technologies will help when developing and specifying standards for AM processes. System integration and cyber implementation can help improve interdisciplinary cooperation in AM processes and implement diverse cloud-based AM information sharing [2]. Metamodels can improve modeling and simulation capabilities, and offer a framework to build predictive models for reliable repeatability [9]. In addition, metamodels can enhance modeling capabilities by facilitating the generation of integrated and composable AM models [9-11].

2. RESEARCH OBJECTIVES AND SCOPE

The main objective in this research is to lay the foundation for building an AM Process Ontology (AMPO). We explore this from the perspective of metal-based processes for AM, starting with powder bed fusion. Powder bed fusion processes can be categorized by four different types of parameters as shown in Table 1: (1) input, (2) control, (3) output and (4) environment.

Input parameters represent powder layer parameters, material properties, and heat source parameters. Control parameters are intentionally changeable parameters for proper execution of an AM process. Output parameters describe information of the final part such as geometric dimensions, surface roughness, and residual stress. Environment parameters represent the peripheral parameters of AM processes. A metamodel can define relationships between these four different categories of parameters and show how various parameters are interconnected [9].

With numerous computational models for AM processes, and the complex interconnections among them, identifying causal connections is a difficult task. An ontology-based metamodel can provide the necessary structure to expose these causal connections – relating inputs to outputs from different modeling views. A well-founded and epistemologically accurate (non-ambiguous) ontology will help when composing models towards accurate and reliable predictive models, with common vocabulary and homogenized data sets.

In this paper, we focus on thermal models for metal-based AM using powder bed fusion. We attempt a classification of the models within this intentionally narrow scope to help visualize the relationships between properties among different thermal models. This is accomplished through an ontology we develop and introduce in this paper. We place a focus on how different types of laser sources affect independent thermal models. The result of the work is described in the following sections.

3. MODELING TAXONOMY

3.1. LASER PHYSICAL MODEL

Laser physical models describe the way in which the source produces a two-dimensional laser irradiation on the powder bed. Idealized laser models have been proposed in the literature to describe the distribution of the surface irradiation. Constant laser models, double ellipsoid laser models and Gaussian laser models are considered in this study. A constant laser beam model may use a simple laser model to irradiate the surface of material $W \times L \times D$ (W, width; L, length; D, depth) [14]. The double ellipsoid laser model is combined with two quadrants of ellipsoid in order to overcome the gap between the calculation and experimental findings of an ellipsoid laser model [15]. A radially symmetrical distribution laser model is provided by a Gaussian laser model, which is often the preferred type of laser source [30]. Each of these is described in the remainder of this section.

Parameters		
Inputs	Powder Layer	relative density, particle shape, particle size and shape distribution, thermal conductivity, absorptivity, reflectivity, emissivity, diffusivity
	Material	viscosity, surface tension, capillary force, conductivity, convectivity, specific heat, melting temperature, evaporation temperature
	Laser	mode (continuous wave, pulsed), wavelength, intensity profile, average power, peak power, beam quality (how well the beam can be focused), polarity
Control	Laser beam	intensity, beam spot size
	Process	scan speed, hatch space, scan strategy
	Layer	thickness, powder density
Output	Part	surface roughness, geometric dimension, porosity, residual stress, microstructure
Environment		Inert gas (Nitrogen, Argon), chamber pressure, ambient temperature, gas flow (rate and direction), surface free energy between the liquid metal and the gas

 Table 1. Parameters for powder bed fusion additive manufacturing [9]

Constant laser model

The constant laser model consists of total absorbed power, length of laser beam (ℓ) , and the width of the laser beam (d). The schematic diagram in Figure 2 shows a constant laser beam along a scanning direction.

$$q = \frac{Total \ absorbed \ Power}{Length(\ell) \ \times \ Width(d)}$$
(1)



Figure 2 Schematic diagram of constant laser beam [14]

Double ellipsoid laser model

The power density distribution of the double ellipsoid has the fractions f_f and f_r , which are in the front and rear quadrants, respectively (see Figure 3). The following equations present power density distribution in the front and rear quadrants.

$$q(x, y, z, t) = \frac{6\sqrt{3}f_f Q}{abc\pi\sqrt{\pi}} e^{\frac{-3x^2}{a^2}} e^{\frac{-3y^2}{b^2}} e^{\frac{-3[z+v(\tau-t)]^2}{c^2}}$$
(2)

$$q(x, y, z, t) = \frac{6\sqrt{3}f_r Q}{abc\pi\sqrt{\pi}} e^{\frac{-3x^2}{a^2}} e^{\frac{-3y^2}{b^2}} e^{\frac{-3[x+\nu(\tau-t)]^2}{c^2}}$$
(3)



Figure 3 Schematic diagram of double ellipsoid laser along the ξ axis [15]

Gaussian laser model

The Gaussian distribution of energy density consists of laser power (P), the absorption coefficient of the laser (η), the effective radius of the laser (r_{eff}), and the beam distribution parameter (d) [16-22] and is given by:

$$q_s = \frac{\eta P d}{\pi r_{eff}^2} e^{\left(-\frac{d(x^2 + y^2)}{r_{eff}^2}\right)}$$
(4)

3.2. THERMAL PHYSICAL MODEL

Various thermal models have been developed and reported in the literature for metal-based AM processes. The most common thermal model is a heat transfer model with utilization of Fourier heat conduction theory [29]. Conservation equations for mass, momentum, and energy are used in mathematical models to compute temperature profiles and melt pool geometry [25].

The classical solution to this problem is found in Rosenthal's model, which describes the temperature distribution in a semiinfinite medium due to a point source traveling with constant velocity [27]. Another physical model addresses the melting and resolidification of two different metal powders [28]. Each model is defined next.

Heat transfer model

Conduction:
$$\rho C_p \frac{dT}{dt} = -\nabla \cdot q(r,t) + Q(r,t)$$
 (5)

Convection: $q_{conv} = h(T_s - T_{\infty})$ (6)

Radiation:
$$q_{rad} = \varepsilon \sigma (T_s^4 - T_{\infty}^4)$$
 (7)

Michaleris et al. [23] use a heat transfer model to calculate temperature history in directed energy deposition (DED). A heat transfer model has temperature (T), time (t), heat source (Q), density (ρ), specific heat capacity (C_p), relative reference coordinate (r) and heat flux (q) [23, 24].

Fluid flow model

Conservation equation for mass:
$$\frac{\partial(\rho u_i)}{\partial x_i} = 0$$
 (8)

Conservation equation for momentum:

$$\frac{\partial(\rho u_j)}{\partial t} + \frac{\partial(\rho u_j u_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\mu \frac{\partial u_j}{\partial x_i} \right) + S_j$$
(9)

Conservation equation for energy:

$$\rho \frac{\partial(h)}{\partial t} + \frac{\partial(\rho u_i h)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{k}{c_p} \frac{\partial h}{\partial x_i} \right) - \rho \frac{\partial(\Delta H)}{\partial t} - \rho \frac{\partial(u_i \Delta H)}{\partial x_i}$$
(10)

Debroy et al. [25] also investigate fluid flow laser welding modeling in DED to compute temperature, velocity of fluid flow and geometry of a molten pool. These equations contain velocity components (u_i, u_j) along the i, j direction; x_i the distance along the *i* direction; effective viscosity (μ); and the source term (S_j) for the j component momentum equation; the sensible heat (h); specific heat (C_p); and the change in enthalpy (ΔH) [25, 26].

Rosenthal-based model

The Rosenthal solution has initial temperature (T_0) , absorption rate (α) , laser power (Q), scanning speed (V), specific heat capacity (c), thermal conductivity (k). It assumes that laser beam moves along x direction [24, 27]:

$$\bar{T} = \frac{e^{-\left(\bar{x}_0 + \sqrt{\bar{x}_0^2 + y_0^2 + \bar{z}_0^2}\right)}}{2\sqrt{\bar{x}_0^2 + \bar{y}_0^2 + \bar{z}_0^2}}$$
(11)

$$\bar{T} = \frac{T - T_0}{\left(\frac{\alpha Q}{\pi k}\right) \left(\frac{\rho c V}{2k}\right)}$$
(12)

$$\bar{x}_0 = \frac{x_0}{2k/\rho cV}$$
, $\bar{y}_0 = \frac{y_0}{2k/\rho cV}$, $\bar{z}_0 = \frac{z_0}{2k/\rho cV}$ (13)

Melting and resolidification in two-component metal powder

Models of melting and resolidification involving two metal powders considers three stages:

Preheating stage:
$$\frac{\partial T_s}{\partial t} = \alpha_s \frac{\partial^2 T_s}{\partial z^2}, z > 0, -\infty < t < t_m$$
 (14)

Melting with shrinkage stage:

$$\alpha_l \frac{\partial^2 T_l}{\partial z^2} = \frac{\partial T_l}{\partial t} + w \frac{\partial T_l}{\partial z}, s_0 < z < s(t), \ t_m < t < t_{sol}$$
(15)

Resolidification stage:

$$\frac{\partial T_l}{\partial t} = \alpha_l \frac{\partial^2 T_1}{\partial z^2}, s_0 > z > s(t), t > t_{sol}$$
(16)

Zhang et al. [28] classified three stages of two different metal powders in powder bed fusion processes. The preheating stage in a powder bed fusion process is governed by the conduction equation. During the melting stage, the governing equation is defined as the period between when the powder starts to melt (t_m) but before solidification begins (t_{sol}) , where w is the velocity in the liquid induced by the shrinkage of the powder bed. After melting stops, resolidification begins with $s_0 = constant$ and w = 0, which is considered the governing equation of resolidification [28].

After having identified the models and the governing equations for these models, we are provided with sets of parameters and the relationships between these parameters. We can use these parameters and relationships to characterize the physical phenomena, in this case thermal phenomena. Different models allow us to characterize the same phenomena in different ways. An ontology allows us to not only capture these differences but also reconcile them through the development of metamodels. We discuss such an approach in the next section.

4. IMPLEMENTATION

4.1. ONTOLOGY IN PROTÉGÉ

Protégé is a widely-used open source ontology development software developed at Stanford University. It can export a file to RDF, OWL, and XML formats. The software can edit knowledge representation systems and manipulate knowledge systems via a graphical user interface. Protégé offers extensible plugins developed by general users, which provide users with a flexible environment [31].

4.1.1 CLASSES AND INDIVIDUALS

Figure 4 shows the hierarchical class structure, individual AM models, and the relationships between individuals. The ontology follows two main classes: (1) **AM_process_parameter** and (2) **Thermal_model**. These are high-level classes in the metamodel, which consists of input, control, and intermediate process parameters.

AM_process_parameter is a super class of information related to controllable input parameters that can be manipulated. An example subclass is **Heat_source**, which can represent several different types of heat sources such as laser, e-beam, and plasma. **Laser power density** is a subclass of heat source.

As discussed in the previous section, published literature mainly concentrates on three different types of laser power densities based on heat flux of constant density, double ellipsoid density, and Gaussian density. The individuals of Laser power density capture these laser heat sources. Heat flux of constant density represents the laser type that keeps constant laser power density distribution. Heat flux of double ellipsoid density represents laser beam that has double ellipsoid type. Heat flux of gaussian density represents Gaussian type of laser, which is the most popular type of laser model.

Thermal_model categorizes the different types of thermal models into single and two powder models. For instance, Single_powder has Heat_transfer, Melting, and Rosenthal_model classes. Melting is associated with several different models such as Buoyancy_effect, Fluid_flow_model, and Maragoni_effect.

Heat_transfer is used to symbolize conventional heat transfer mechanisms such as conduction, convection, and radiation. The classes **Conduction**, **Convection**, and **Radiation** represent independent mathematical models with their own parameters as individuals.

Classes of **Melting** address the melting of powders by physical phenomena in powder bed fusion AM processes. **Buoyancy_effect** represents an upward force by the fluid. In the case of **Fluid_flow_model**, conservation equations, such as energy, mass and momentum conservation, are used for numerical models. **Maragoni_model** is the mass transfer caused by a surface tension gradient. **Rosenthal_model** represents a widely used model in welding, providing analytical solutions of moving heat sources.

The **Two_powders** class captures a two-component metal powder with significantly different melting points and integral approximation solutions in laser powder bed fusion, considering three different stages such as **Preheating_stage**, **Melting with shrinkage stage**, and **Resolidification stage**.





Figure 5. NavigOwl visualization of laser models

4.2. NAVIGOWL VISUALIZATION

After having developed the ontology in Protégé, we use NavigOwl, an ontology visualization tool specialized for exploring and showing whole role-relation hierarchies of a concept [11]. The NavigOwl utilizes RDF/OWL ontology files and follows a power law-based ontology visualization algorithm. The aim of using ontology visualization is to draw a simple canvas. In this respect, NavigOwl is pertinent to visualization. An ontology has several different panels such as classes, object properties, data properties and individuals. Colored nodes with different panels are visible to researchers interested in finding relationship between nodes.

Visualization of the laser models is given in Figure 5. Yellow and purple circles indicate classes and individuals, respectively. Individuals contain information about physical parameters such as laser power, ambient temperature, and wavelength. Each link represents a relationship. The size of the nodes is proportional to the number of relationships a node has (degree) and differentiates prominent and important nodes from trivial nodes. NavigOwl distinguishes the relationships between classes and individuals in metamodels.

We can see in Figure 5 that the three different types of laser heat sources are influenced by their own parameters and each have an influence on heat flux. Heat flux affects conduction, convection, and radiation in the heat transfer model, and also affects the conservation equation for energy in a fluid flow model. When it comes to heat transfer and fluid flow models, material density, specific heat capacity, thermal conductivity and time are parameters shared in the two models do not appear to have high relevance based on the ontology visualization. Use of this visualization strategy can help identify relationships and interconnectivity between different AM models and their parameters. An example application is given in the next section.

5. APPLICATION OF THE METAMODEL

Figure 6 shows relationships between the Gaussian density laser model and heat transfer models, with a schematic example and network depicting a set of nodes shared by an arc. Yellow colored nodes represent classes, and purple colored nodes represent physical parameters for AM. A node can be associated with more than one node, and the size of node is proportional to the number of connections linking to other nodes. When developing metamodels, it is desired to create and identify larger nodes, therefore generalizing specialized parameters or concepts and supporting their reconciliation.

As shown in Figure 6 the metamodel illustrates links between laser and thermal models. The heat transfer model consists of conduction, convection, and radiation models which are associated with a generated heat flux from laser heat sources. Heat flux is related to different laser density models such as Gaussian and double ellipsoid types, where each laser density type is subject to its own physical parameters. For instance, Heat flux of Gaussian density is mainly influenced by five different individuals this example: in (1)Beam distribution parameter, (2) Absorbed laser power, (3) Effective radius of laser beam, (4) Coordinate(x), and (5) Coordinate(v).

6. CLOSING REMARKS AND FUTURE WORK

This paper identifies relationships between AM modeling parameters with respect to different types of laser models and thermal models for metal-based AM with visualization in Protégé. Different types of laser beam models yield different heat fluxes, which impact the temperature in AM processes and corresponding thermal models. Likewise, thermal models also have different structures and diverse properties, as shown by the examples reviewed in this paper. Building a framework of metamodeling for laser and thermal models is an initial and essential step for a comprehensive understanding of metal-based AM processes as a whole. A better understanding of the models and reconciliation of their data sets makes it possible to gain insight into the physical process of AM.

To leverage AM modeling techniques towards improved reliability and fabrication repeatability in AM, data reconciliation and metamodels become necessary. It is this reconciliation that is of the greatest interest, as process variability can quickly lead to heterogeneous data sets. Bv decomposing processes into sub processes, we can segregate data sets and models to isolate sub-domains with the greatest variability. We can then look to augment these isolated data sets with additional data and clarity in attempt to enhance the overall model. We discuss how our ontology-based approach can provide a fundamental platform for building advanced models and simulations for AM processes. Our initial implementation investigates laser and thermal models, and future work includes development and expansion of AM metamodels by linking mechanical and microstructure models. An expanded ontology will provide information about the interrelationships between heat source, thermal history, microstructure, and mechanical properties.

The results of this ontology study have not yet addressed the different characteristics of materials fabricated through AM processes. Although this research can explain the specific parts of the metamodel in metal-based AM, a single study cannot adequately cover the complete metamodel. Therefore, further studies are needed to demonstrate how laser and thermal models relate to microstructure of materials and the geometry of produced parts, given the existing interrelations between microstructure, mechanical properties, residual stress, and geometry [24]. In this regard, research on microstructure can help bridge the gap between laser and thermal models and mechanical properties of AM parts.



Figure 6. NavigOwl visualization of classes and individuals between Gaussian beam and heat transfer

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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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