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Modeling of additive manufacturing processes for metals: Challenges and opportunities

M.M. Francois [a,*], A. Sun [b], W.E. King [c], N.J. Henson [a], D. Tourret [a], C.A. Bronkhorst [a], N.N. Carlson [a], C.K. Newman [a], T. Haut [a], J. Bakosi [a], J.W. Gibbs [a], V. Livescu [a], S.A. Vander Wiel [a], A.J. Clarke [a], M.W. Schraad [a], T. Blacker [b], H. Lim [b], T. Rodgers [b], S. Owen [b], F. Abdeljawad [b], J. Madison [b], A.T. Anderson [c], J-L. Fattebert [c], R.M. Ferencz [c], N.E. Hodge [c], S.A. Khairallah [c], O. Walton [c]

[a] *Los Alamos National Laboratory, USA*
[b] *Sandia National Laboratories, USA*
[c] *Lawrence Livermore National Laboratory, USA*

1. Introduction

With the technology being developed to manufacture metallic parts using increasingly advanced additive manufacturing processes, a new era has opened up for designing novel structural materials, from designing shapes and complex geometries to controlling the microstructure (alloy composition and morphology). The material properties used within specific structural components are also designable in order to meet specific performance requirements that are not imaginable with traditional metal forming and machining (subtractive) techniques.

Modeling and simulation will play a critical role, in this new era, to enable enhancements to traditional trial and error approaches for the design and optimization of components and materials. Modeling and simulation will also advance our capability to quantify the influence of process variables on resulting component properties. It can help both from a fundamental understanding of the underlying physical processes and enable accelerated design to reduce the qualification cycle of additive manufactured parts.

Current modeling and simulation tools used to simulate materials processing are being extended to model additive manufacturing. Models are needed at multiple length scales to account for the structural details of this new class of materials and to understand the basic physical processes that are active in the performance response of these materials. Models at multiple length scales will enable the development of the dominant physics basis within macro-scale models for use in component performance simulations. This includes an elasto-plastic representation to allow prediction of the propensity for damage in these components – a long term endeavor. Constitutive equations commonly used for standard casting processes do not always provide an appropriate description for additive manufacturing, as suggested by experimental measurements [1,2]. Further multiscale model and algorithm developments are needed that will incorporate knowledge of the microstructure within the macro-scale continuum codes on both the processing (solidification) and solid mechanics sides.

The microstructure of materials that results from the solidification process determines the material properties (such as its response to deformation). Fig. 1 illustrates the integration needed in modeling and simulation to allow the connection between performance and process through knowledge of the microstructure and properties of the material. The needs for and benefits of a process modeling and simulation capability have been detailed in several roadmaps for additive manufacturing [3–6].

In this article, we review the challenges and opportunities that we are facing in the modeling and simulation of additive manufacturing processes for metals and the predictive representation of their mechanical performance at the different scales. This article is divided into five sections in which we highlight the current modeling efforts taking place at the U.S. Department of Energy National Nuclear Security Administration (NNSA) Laboratories: process modeling, microstructure modeling, properties modeling, performance and topology and process optimization. All these various modeling developments at different scales and regimes are necessary in order to move toward an integrated computational approach of process-structure-properties-performance that will ultimately enable the engineering and optimization of materials to specific performance requirements.

2. Process modeling

Two main technologies exist for additive manufacturing of metals: powder-bed and directed energy deposition. In powder-bed technology, a thin layer of metallic powder (20–100 μm) is deposited on a flat surface and then melted using a laser beam according to computer-programmed patterns. The process repeats itself layer by layer with varying laydown patterns and topologies per layer until the part is completed. The remaining powder is then blown and recycled. Laser powder bed fusion additive manufacturing is an inherently multiscale process: material transformations take place locally (O(10–100 μm)) over short times O(10 ms), but parts

* Corresponding author.
E-mail address: mmfran@lanl.gov (M.M. Francois).

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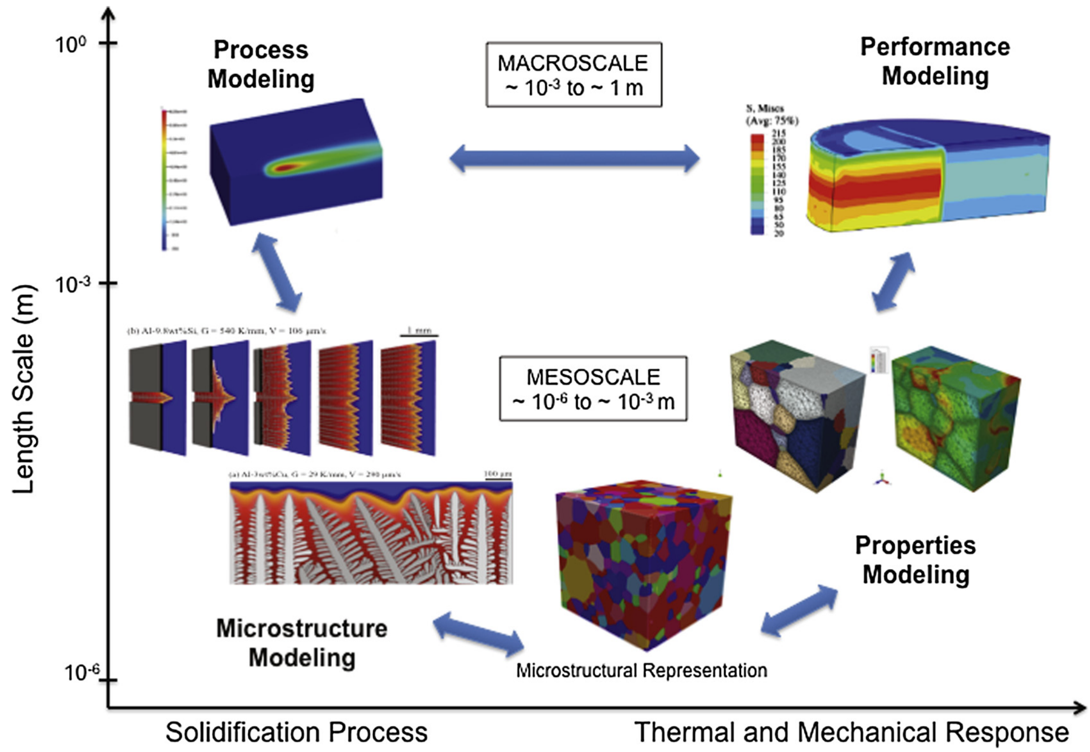

Fig. 1. Illustration of the envisioned integrated process-structure-properties-performance modeling and simulation approach and associated length scales.

are $O(10\ \text{cm})^3$ and take O(hours-days) to build. This calls for an approach using multiple coupled models.

In the direct energy technology, either powder fed or wire fed, the material deposition is localized and occurs at the same time as the laser heat deposition. Typical laser powers are of the order of $O(100\ \text{W})$, beam speeds of O(mm/s) and cooling rates can reach 10^2–10^4 K/s [7–9]. These parameters as well as the powder (or wire) composition will affect the resulting microstructure and residual stresses in the part. Determining defects and residual stresses in the part are what process modeling at the macro-scale can achieve. In addition, we would eventually need to predict the various grain morphologies and crystallographic orientations as well as grain size distributions as a function of position in the part and have microstructure-aware solidification models.

At the macro-scale, simulations of solidification processes are achieved using Computational Fluid Dynamics (CFD) software [10] and resulting residual stresses from solidification are typically computed using Finite-Element Analysis (FEA) software [11,12]. CFD software solves a system of non-linear partial differential equations that represents the motion of fluids, species diffusion and phase changes and ensures mass, momentum and energy conservation. Finite-element analysis software is used for thermo-mechanical modeling during processing solving the coupled governing equations for heat transfer and solid deformation. Please note that our approach is pursued in the context of large scale and high performance computational resources available at DOE national laboratories.

2.1. Direct energy deposition

Simulation of direct energy deposition requires modeling a moving heat and mass source that represent the addition of heat (coming from the laser or electron-beam) and mass coming (from the powder or wire feed) as the part is being built. Such simulation will increase our understanding of the effect of the temperature history, melting-solidification cycles, various scan patterns effects and final residual stress state.

Truchas, a continuum thermo-mechanical modeling tool [13], originally designed for the simulation of casting processes, is being extended to simulate directed energy deposition additive manufacturing processes. Fig. 2a illustrates the simulated melt pool region during a single weld pass in a 304L stainless steel. Fig. 2b shows the modeling of mass and energy deposition in Truchas.

One of the major challenges in CFD modeling of such processes is the description of surface tension and its local variations with temperature and chemical composition. These variations are at the origin of Marangoni flow within the liquid, which significantly affects the shape and depth of the melt pool. Accurate simulation of the melt pool geometry and the possible gas entrapment at the origin of voids and defects are crucial to the prediction of the final quality of the parts. Therefore, simulation tools like Truchas are expected to play a key role in refining/optimizing processing conditions, such as the laser power and its traveling speed to design and produce optimized parts.

2.2. Powder bed system

Simulation at the scale of the powder has the potential to increase our understanding of the physics of the additive manufacturing process, contribute to improving the process, provide insight when extrapolating beyond current experience, and contribute to improving the design of laser powder bed fusion additive manufacturing machines. Powder scale models capture the details of laser interaction with the powder, including vaporization effects, that can be used to determine the net laser energy input for the part scale models and to investigate such phenomena as spattering and denudation. These models give temperature and time histories of the melt pool, with applications to real-time process diagnostics and microstructure development. Powder scale models can also be used to study issues of surface finish and part density.