# Computational Materials for the Design and Qualification of Additively Manufactured Components

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NASA is developing next-generation computational materials capabilities to support the qualification of additively manufactured metallic structural components for aerospace applications. The quality of parts produced by the additive manufacturing process directly depends on a wide range of process parameters, which includes the build conditions and feedstock properties. The present computational materials research aims to develop a fundamental understanding for the dependence of the part properties and performance on the process parameters and to apply that understanding towards efficient qualification practices. Integrated multiscale modeling methods allow the prediction of the process-structure-property relationships including the effect of defects. This talk will primarily focus on the powder bed fusion process. The presentation will include discussion of in-situ monitoring, process to microstructure linkages including residual stress, and microstructure to performance linkages. The computational materials research for additive manufacturing processes will enable efficient and accurate design, manufacture, and certification of future aerospace flight systems.

## Introduction

Although additive manufacturing (AM) technology has recently experienced considerable growth and publicity for its potential to significantly transform the manufacturing industry, the promise of AM is limited in application due to a lack of confidence in the part quality. Improvements in material properties, consistency, and process control are necessary in order for AM to realize the advertise potential of improved performance, reduced cost, and increased manufacturing speed. Additionally, the application of AM to fracture-critical flight components requires extensive qualification efforts.

Additive manufacturing encompasses a variety of materials including metals, polymers, and ceramics and processes including powder bed, blown powder, wire fed, laser, and electron beam. The part quality and consistency depends on the numerous process specific parameters that are selected or adjusted for each component. While the focus here is the laser powder bed fusion (LPBF) process for metallic AM, many of the approaches are applicable to a wide range of materials and manufacturing processes. The LPBF parameter space consists of laser parameters, scanning strategy, feedstock, part geometry, and machine conditions. The selection of process parameters determines the resulting microstructure and therefore component properties. Currently, various libraries of process parameters exist for a given machine and material which have been determined through trial and error testing by AM suppliers or individual laboratories with additional testing required for each new part geometry or powder supply. An integrated computational materials engineering (ICME) approach will reduce the amount of physical testing and will inform the design engineers regarding the detrimental performance expected for specific process parameters (Turner 2015).

NASA is actively developing AM rocket engine components for human spaceflight. To address the immediate need for a consistent framework specific to the production and evaluation of LPBF processes, standards have been released by Marshall Space Flight Center (MSFC 2017) for material, process control, personnel training, inspection, and acceptance requirements. Concurrently, an ICME approach to the design and qualification of aerospace AM materials and their components is being developed at NASA and provides a path towards rapid manufacturing and qualification. Improved control and understanding of the AM process offers improved consistency and more complex design such as multiple alloys and functionally graded material components. When combined with in-situ process monitoring, computational modeling enables the development and integration of manufacturing process capabilities and constraints as well as qualification considerations such as inspection requirements into the component design.

**Computational Modeling of the Process**

Process modeling aims to develop an understanding of the relationship between the process parameters, feedstock, microstructural and porosity evolutions, and the resulting mechanical properties by solving the governing equations for the physics of the process. Determination of the temperature history, deformations due to residual stress, microstructure evolution, and porosity are among the goals of current process simulation efforts.

Modeling the AM process requires a multiscale approach to accurately account for the physics at the various length scales from microstructure to component scale. An accurate temperature history and melt pool geometry are necessary to understand the microstructure, defect formation, and residual stress formation. The temperature history is predicted by numerical models at varying levels of fidelity. Various physics are incorporated to improve the model accuracy and include melting, evaporation, fluid flow, recoil pressure, powder packing density, and surface tension. Due to accuracy and computational resource requirements, the thermal models are generally restricted to a low number of scan tracks and powder layers. Simulation of residual stress formation requires a scale-up to efficiently account for the numerous layers in an AM build. A promising approach for predicting residual stress is the modified inherent strain method, which computes the inherent strain at the scan track scale and imposes the inherent strains in a layer by layer fashion to a part scale mechanical analysis (Liang 2018). Phase-field and kinetic Monte Carlo models are implemented to simulate grain structures dependent on feedstock and temperature history.

Two sources of porosity during the LPBF process are lack of fusion and keyholing. The melt pool transitions from conduction mode to keyhole mode for increased laser power and reduced scan speed. Keyhole mode occurs when a vapor cavity forms with a high aspect ratio of depth to width as compared to conduction mode (Trapp 2017). In contrast, lack of fusion occurs when insufficient power and overlap of successive melt pools is applied to fully melt the powder. A balance exists for avoiding lack of fusion and keyhole porosity which is determined by the selected process parameters (Tang 2017).

Porosity cannot be completely avoided, and the impact of the porosity on part performance becomes application dependent. Micromechanical simulations quantitatively characterize the influence of porosity and other heterogeneities in the microstructure on the mechanical behavior of parts produced by LPBF.

Porosity is embedded into process-specific microstructure models, and the heterogeneous strain localization in the vicinity of the porosity is solved as a function of the pore shape, size, density, and proximity to the free surface.

**In-situ Process Data**

For the design and qualification of AM components, experimental data is required to capture critical events and behavior during the manufacturing process. Powder bed systems are being equipped with various sensors and measuring devices to record data during the manufacturing process. System monitoring provides critical data necessary to understand process events, perform feedback control, diagnose machine operation, and validate computational models. Key process measurements include temperature history, melt pool dimensions, and defect formation. Collection of in-situ data provides a component build history which can identify critical events which occur during the process regarding part quality.

Dynamic x-ray radiography (DXR) being performed at the Argonne National Laboratory Advanced Photon Source provides high speed cross-section videos of the laser powder bed fusion process (Sun 2017). The real time imaging provides data relative to the laser position including melt pool dimensions, key-hole behavior, solidification rate, and porosity formation. Data from the DXR experiments helps characterize the melt pool and solidification behavior for various feedstock compositions and baseplate material as well as varying laser parameters.

**Summary**

Computational modeling supports the qualification efforts necessary to realize the full potential of AM for designing and manufacturing aerospace components. A large design space exists for AM, and an ICME approach to process and component design supports qualification efforts through improved process understanding and control for application and material specific needs. Leveraging simulation tools that assist in choosing parameters for process control and designing AM specific components leads to microstructures that help attain and exceed design specifications. Micromechanical simulations characterize part performance for process-specific microstructures including the effect of defects. Integrated computational modeling and in-situ process monitoring efforts provide a path towards accelerated design and qualification of aerospace components.

**References**

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