BUILDING THE FUTURE

MODELING AND UNCERTAINTY QUANTIFICATION FOR ACCELERATED CERTIFICATION

Livermore technician Manuel Iniguez removes a finished component from the build chamber of a selective laser-melting (SLM) additive manufacturing (AM) machine. (Photo by George Kitrinos.)

Advanced manufacturing methods have motivated Livermore researchers to rethink how to better qualify components.

IN industries such as aerospace, defense, and medicine, the manufacturing processes and materials used to produce critical components must be formally qualified to ensure they perform to specification, as failure could prove disastrous. The extensive empirical testing and evaluation required to develop a material and qualify a component often encompass many thousands of individual tests, at a cost of millions of dollars and 5 to 15 years of effort. Later, even a minor manufacturing process change could necessitate complete requalification. This traditional qualification approach makes it difficult for producers to leverage the speed, flexibility, and cost savings that advanced techniques such as additive manufacturing (AM) offer. (See *S&TR*, September 2014, pp. 20–23.) AM refers to a category of manufacturing processes in which a polymer- or metal-based material is added layer by layer in concordance with a virtual blueprint. (See *S&TR*, March 2012, pp. 14–20.) AM methods can be used to create objects with shapes or properties that are difficult or impossible to achieve through traditional subtractive manufacturing methods such as machining.

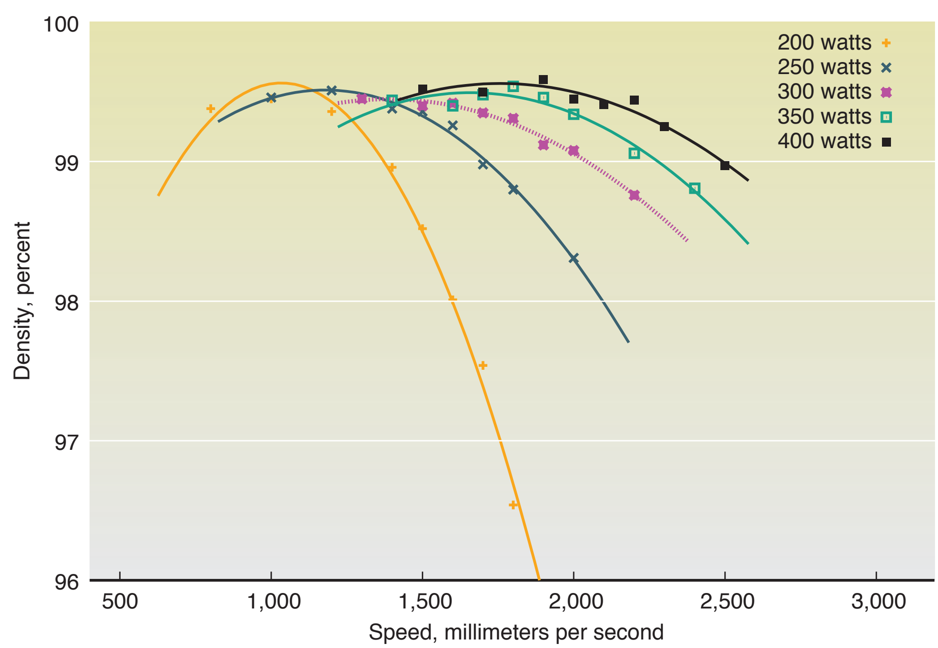
AM can also speed the development of complex designs, accelerating the development cycle and enabling customization. However, to realize AM's full potential, Livermore scientists posit that the processes to qualify components and certify systems must also be accelerated. "One of the most serious hurdles to the broad adoption of additive manufacturing of metals is the qualification of additively manufactured parts," says materials scientist Wayne King. "At this time, concern is focused on the quality of the final product." King leads Livermore's Accelerated Certification of Additively Manufactured Metals (ACAMM) Initiative, which began in late 2012. ACAMM is supported by Laboratory Directed Research and Development (LDRD) funding and builds on Livermore's foundational capabilities and previous successes in areas such as materials synthesis, predictive simulation, advanced manufacturing, and materials characterization.

Rather than undertaking exhaustive experimentation, King's team borrows a formula that has proven highly effective for stockpile stewardship work: modeling and simulation paired with targeted experiments and guided by data mining and uncertainty quantification (UQ). "With deep scientific knowledge, we develop more confidence in the process, and this confidence leads to qualification," says King. "High-performance computing plays a key role. We have used it to support certification of the stockpile by simulating systems and building confidence, and we believe high-performance computing can help us in a similar way in the metal AM arena." In turn, the results of this LDRD project may, with additional development effort, be applied to Livermore's nuclear stockpile mission. Nuclear engineers and AM experts are presently exploring how AM methods could benefit weapons refurbishment endeavors. (See the article beginning on p. 4.)

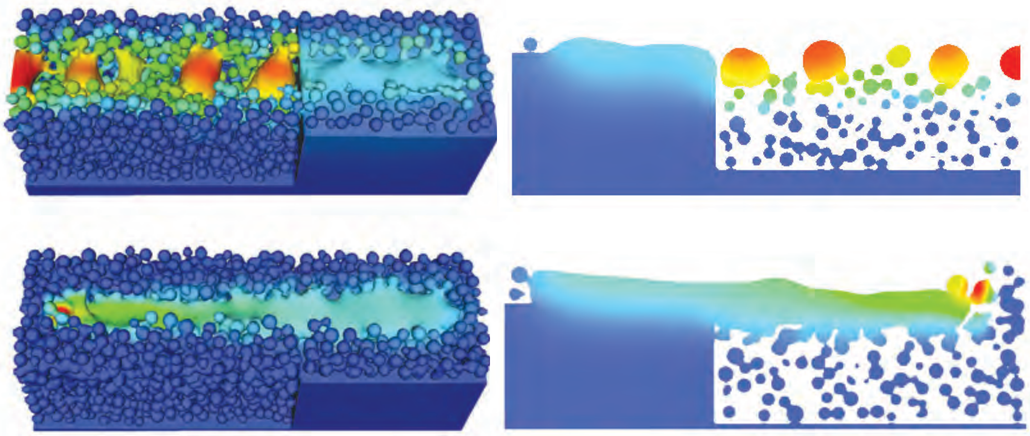
In the first two years of the project, King's team of computational experts has built and begun testing platforms for its multiscale modeling and data-mining efforts. With these platforms, the researchers are progressing toward understanding and optimizing the rapid heating, melting, cooling, and solidification processes at the heart of metal AM.

Less Trial and Error

For selective laser-melting (SLM) AM, Livermore researchers are using data-mining techniques to efficiently hone the optimal process parameters that result in parts with desired properties. With SLM, a high-energy laser beam fuses metal powder particles, layer by layer, to produce a three-dimensional (3D) part. Some SLM applications require parts with greater than 99 percent density, because voids, or pores, weaken



Livermore researchers have shown that modeling combined with a set of experiments is an efficient and reliable method for determining AM process parameters. This approach has helped them understand how various laser power and laser-scanning speeds during SLM influences the density of the part produced. For certain applications, parts with greater than 99 percent density are needed because of their superior strength.



Powder-scale modeling with the code ALE3D provides an efficient avenue for understanding how to adapt process parameters to build a part with an overhang geometry. In the top scenario, both the laser power and scan speed are high, a combination that produces an undesirable balling effect. By lowering the scan speed and power (bottom scenario), a better build can be achieved.

the material and cause parts to fail. Unfortunately, the sheer number of process parameters that influence the quality of the material produced—more than 130—can make it difficult to determine the best settings without many rounds of experimentation. Some of these parameters include laser power, laser-scanning speed, distance between the laser scan lines, scanning pattern, and powder-layer thickness.

A team of researchers, led by computer scientist Chandrika Kamath, has used a combination of simulations and experiments to streamline the optimization process and identify variables likely to influence the density of stainless-steel parts. The team began by performing more than 500 simple, computationally efficient laser-melting simulations to pinpoint the parameters that played the largest role in determining the dimensions of the melt pool, which is the pool of liquid formed when the laser melts the metal powder particles. Using data-mining techniques to uncover patterns in the simulation results, the researchers found that laser power and scanning speed were the most crucial parameters. They also identified ranges of power and speed that would result in melt pools of the right depth. "We mined the simulation output to identify important SLM parameters and their values such that the resulting melt pools are just deep enough to melt through the powder into the substrate below," says Kamath.

Focusing on just these two parameters in the physical experiments enabled the team to reduce the number of experiments necessary to achieve high-density parts. The researchers first used a subset of speed and power values to perform basic single-track experiments, in which a laser creates a series of tracks in a metal plate. They found that when the speed was too low, the laser drilled into the material and produced pores, reducing the metal's density. Too high a speed generated insufficient melting. Once equipped with a subset of values deemed most likely to produce the right melting conditions, the team printed a series of small steel pillars with more than 99 percent density on the first attempt. The experiments also yielded significant data on the role of laser power in particular. For the stainless-steel powder under study, the density remained high over a wider range of scanning speeds at higher powers than at lower powers, which suggests that higher powers offer greater flexibility when choosing process parameters.

This effort helped demonstrate that computer simulations, data mining, and a select set of experiments can be used to quickly and reliably determine process parameters. The team expects that a similar approach could be used to optimize other properties of a manufactured part or other materials. Furthermore, data mining is just one tool that helps the researchers make efficient use of the vast quantities of data that experiment and simulation are producing. In the future, a growing role will be played by UQ techniques as they are used to understand how uncertainties in inputs, such as powder quality and laser power and scanning speed, will affect the properties of parts manufactured using AM.

Micrometer-Scale Insights

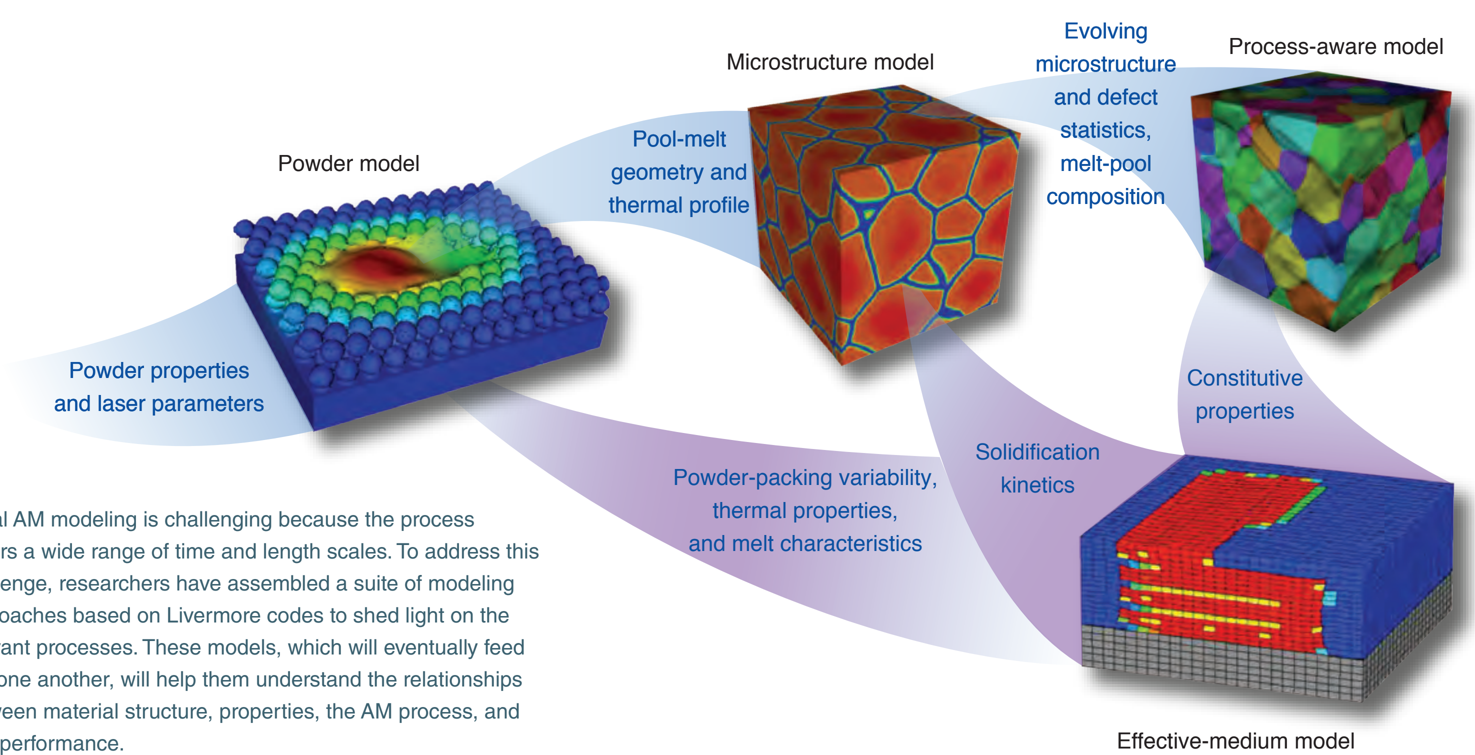
Since the cessation of nuclear testing in the early 1990s, the Laboratory has focused particular attention on developing predictive models for regimes where experimental data are not always available. These tools are aiding the ACAMM team in developing a multiscale predictive modeling capability based on physics first principles and validated through physical experiments. Modeling AM processes and predicting AM part performance can be challenging, because the materials science involved is complex and covers a broad range of time and length scales. Such modeling may be computationally intensive but is possible with Livermore's exceptional high-performance computing (HPC) resources. Researchers use information provided by these models to improve AM processes, obtain desired microstructures, and reduce manufacturing errors. Two models, based on Livermore-developed codes, have already shown significant promise.

As the range of AM applications grows, so do the variety of metals Livermore researchers desire to additively manufacture. Some of these materials may never have been tested in AM machines, while others may not meet the machine manufacturer's specifications. For instance, a powder with a more varied particle size than recommended may be much cheaper, but it could also have performance implications. Engineer Andy Anderson and physicist Saad Khairallah have developed a model to help researchers understand whether a given powder can be processed by AM and, if so, what are its optimal processing conditions. Powered by Livermore's massively parallel multiphysics code ALE3D and HPC resources, the tool is the first high-fidelity, 3D powder-scale model of an SLM process.

This model resolves the melting and solidification of individual powder particles on submicrosecond timescales. "The simulations reveal that the surface-tension effects on topology and heat transfer drive the SLM process," says Anderson. The researchers observed behaviors in the melted region that resembled Plateau–Rayleigh instabilities, such as those that occur when a thin water stream breaks into droplets. These instabilities can occur at high laser speeds and create undesirable effects such as surface roughness and disconnected balls of material, both of which were observed in some experiments.

Khairallah and Anderson used the powder model to better understand the main physical processes occurring and to optimize process parameters. They found that for a fixed laser power and at high laser-scan speeds, less heat is deposited, and therefore the particles do not fully melt. This scenario can cause surface roughness and porosity to increase. Lower laser-scan speeds enable the particles to melt completely and produce conditions favorable for achieving the low porosity, smooth surface, and high density that the researchers desire. However, if too much heat is deposited, the material can enter a keyhole regime, where the laser drills into the sample, causing extensive material evaporation and creating plasma.

These simulations complement Kamath's efforts to efficiently optimize process parameters. She is analyzing the data from the simulations to understand how to create parts with smoother surfaces. Notes Khairallah, "We were surprised and pleased the first iteration of our model captured the essential characteristics of the melt track. Now that we understand the magnitude of our



Metal AM modeling is challenging because the process covers a wide range of time and length scales. To address this challenge, researchers have assembled a suite of modeling approaches based on Livermore codes to shed light on the relevant processes. These models, which will eventually feed into one another, will help them understand the relationships between material structure, properties, the AM process, and part performance.

approximations, we can add more physics effects to the model.”

Building a Virtual Part

While the powder model looks at a single layer of metal powder and its interactions with the laser, the Livermore-developed effective-medium model is intended to computationally build a complete part and predict material properties such as residual stress and part characteristics such as unwanted distortions. The development team based this model on the Livermore engineering code Diablo, which is used to look at slowly evolving processes. Simulations cover a time period as long as several hours and a length scale of centimeters.

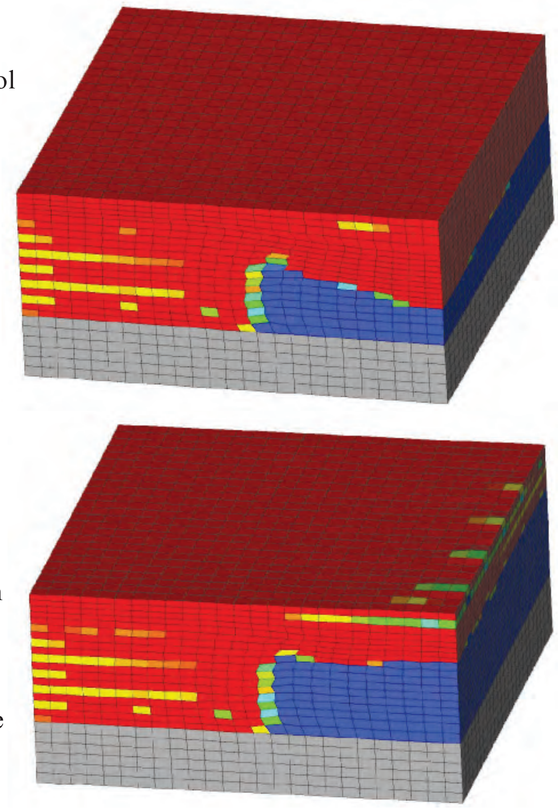
The effective-medium model has been successfully used to simulate several phenomena. Computational engineer Bob Ferencz explains, “We’re interested in studying effects such as the cyclical shrinking a material undergoes as its layers are heated to thousands of degrees and then cooled. We have found the material near the melt layer, including the fused layers beneath, undergoes significant thermal processing over time. We need to know how that reworks the material.” By sharing their temperature data with material scientists, Ferencz and his team hope to gain insight into how these temperature fluctuations influence the metal’s microstructure, which could in turn enhance the model.

Early studies focused on modeling just a cubic millimeter domain of powder, which equals about 20 layers of particles. Even this small scale has shed light on problems such as rough surfaces in overhang regions. An overhang is a downward-facing surface of a part that is supported only by underlying unconsolidated powder as opposed to melted and solidified metal. Creating overhang features with SLM often results in an undesirable finish on the underside that necessitates further machining. Using overhang construction simulations, computational engineer Neil Hodge found that an uneven surface forms when the laser melt pool penetrates the previously unmelted layers. He demonstrated through further simulations that adjusting the laser power several times over the course of part production could mitigate excessive melting. With the acquisition of a sophisticated SLM machine from Germany’s Fraunhofer Institute for Laser Technology, Livermore researchers soon will be able to verify simulation results and experiment with laser power modulation during the printing process.

Ferencz’s team also had some initial success in modeling residual stresses in centimeter-scale parts. These stresses are induced by the laser-melting process and change with the part’s subsequent removal from the base plate on which it was built. Understanding these stresses is important for predicting part performance and improving the SLM process. The researchers modeled stresses in prism- and L-shaped stainless-steel test objects both before and after the objects were removed from their base plates.

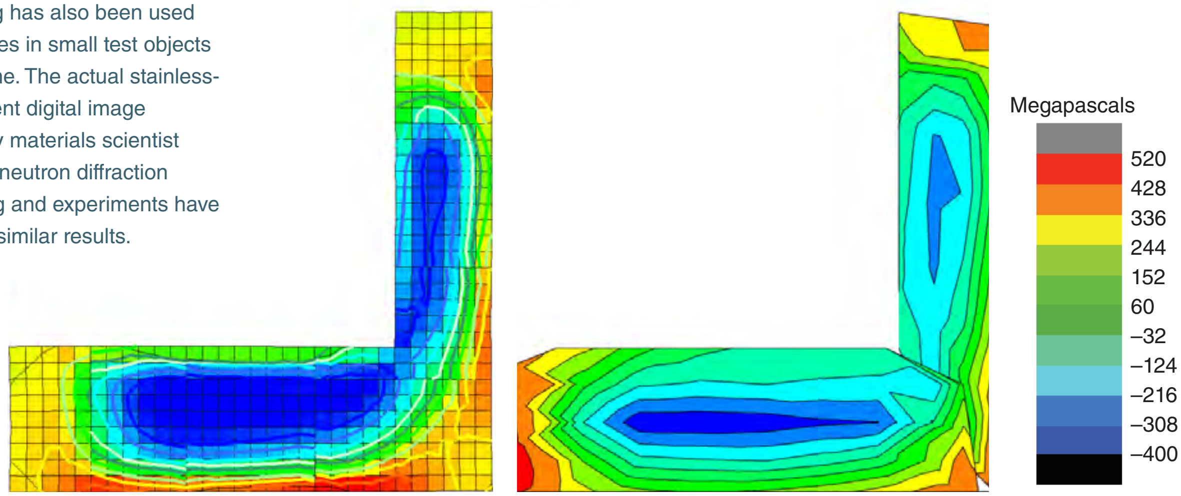
For comparison, the actual parts were evaluated experimentally using nondestructive neutron diffraction at Los Alamos National Laboratory. The experimental results provided information on residual stress. Livermore materials scientist Amanda Wu also used digital image correlation to study the parts. This technique involves first painting a speckled pattern on the surface of a part and then photographing the part with a pair of cameras as the part separates from its base plate. Wu analyzed the image series to determine how much the material had distorted from the residual stresses.

The team found that predicted and actual stresses were quite similar. Given



Livermore researchers have used Diablo part-scale modeling to understand and correct the formation of uneven surfaces in overhang regions. (top) When the laser sweep proceeds at a uniform speed and power, it tends to produce excessive melting and consolidation (red) beneath the intended overhang, causing previously unprocessed powder (blue) to fuse and form a rough downward-facing surface. (bottom) By modulating the power, the simulations suggest this problem can be mitigated and a more even surface produced.

(left) Part-scale modeling has also been used to predict residual stresses in small test objects such as this L-shaped one. The actual stainless-steel test object underwent digital image correlation, performed by materials scientist Amanda Wu, and (right) neutron diffraction measurements. Modeling and experiments have achieved encouragingly similar results.



that modeling at this larger scale required simulations of "metalayers" rather than individual layers to speed up the simulation, the researchers were pleased to find that they were still able to reasonably capture stresses in the parts. They have now begun modeling residual stress in parts where a larger percentage of the surface area touches the base plate, which poses a greater challenge.

Diagnostics Complement Modeling

Future efforts will tie in the powder and effective-medium models with two others—a microstructure model designed to predict the microstructures that develop during the AM process and a process-aware model that predicts temperature and behavior for the effective-medium model. Ultimately, these models will be used to connect the AM process with the resulting material microstructure and properties and accurately predict the performance of the material.

While the deep understanding of the AM process that simulation affords is essential, it is not enough for qualification. The ACAMM team will also be integrating sensors and diagnostics into the Fraunhofer SLM machine to ensure that the process developed through modeling and simulation proceeds as planned during part production. Once process-monitoring capabilities are fully established and coupled with a mature multiscale model, it may become possible to qualify each part as it is built.

—Rose Hansen

Key Words: Accelerated Certification of Additively Manufactured Metals (ACAMM) Initiative, additive manufacturing (AM), data mining, digital image correlation, effective-medium model, high-performance computing (HPC), Laboratory Directed Research and Development (LDRD) Program, neutron diffraction, powder model, predictive modeling, process monitoring, selective laser melting (SLM), uncertainty quantification (UQ).

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