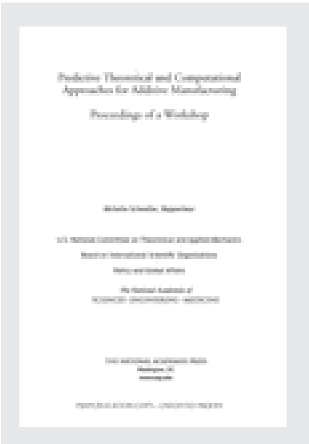

Predictive Theoretical and Computational Approaches for Additive Manufacturing: Proceedings of a Workshop

DETAILS

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AUTHORS

Michelle Schwalbe, Rapporteur; U.S. National Committee on Theoretical and Applied Mechanics; Board on International Scientific Organizations; Policy and Global Affairs; National Academies of Sciences, Engineering, and Medicine

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Proceedings of a Workshop

Michelle Schwalbe, *Rapporteur*

U.S. National Committee on Theoretical and Applied Mechanics

Board on International Scientific Organizations

Policy and Global Affairs

The National Academies of
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REVIEWERS

This report has been reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise, in accordance with procedures approved by the National Academies of Sciences, Engineering, and Medicine's Report Review Committee. The purpose of this independent review is to provide candid and critical comments that will assist the institution in making its published report as sound as possible and to ensure that the report meets institutional standards for quality and objectivity. The review comments and draft manuscript remain confidential to protect the integrity of the process.

We wish to thank the following individuals for their review of this report: Michael Gorelik, Federal Aviation Administration; Lonnie Love, Oak Ridge National Laboratory; Amit Misra, University of Michigan; Edwin Schwalbach, Air Force Research Laboratory; and Tarek Zohdi, University of California, Berkeley.

Although the reviewers listed above have provided many constructive comments and suggestions, they were not asked to endorse the content of the report, nor did they see the final draft before its release. The review of this report was overseen by Robert Schafrik (Retired), General Electric Aviation. Appointed by the National Academies, he was responsible for making certain that an independent examination of this report was carried out in accordance with institutional procedures and that all review comments were carefully considered. Responsibility for the final content of this report rests entirely with the rapporteur and the institution.

Wing Kam Liu
Chair, Planning Committee

Contents

1

Introduction

Additive manufacturing (AM) methods have great potential for promoting transformative research in many fields across the vast spectrum of engineering and materials science. AM is one of the leading forms of advanced manufacturing which enables direct computer-aided design (CAD) to part production without part-specific tooling. Conventional applications, such as tooling, low production parts, biomedical devices and implants, aerospace components and rapid prototyping, all benefit from the flexibility that AM provides. The technology likewise can enable material design and development of metamaterials. While experimental workshops in AM have been held in the past, this workshop uniquely focused on theoretical and computational approaches and involved areas such as simulation-based engineering and science, integrated computational materials engineering, mechanics, materials science, manufacturing processes, and other specialized areas. The full statement of task is shown in Box 1-1.

WORKSHOP OVERVIEW

On October 7-9, 2015, the National Academies of Sciences, Engineering, and Medicine convened a workshop of experts from diverse communities to examine predictive theoretical and computational approaches for various AM technologies. A planning committee (shown on p. v) was established to identify specific workshop topics, invite speakers, and plan

BOX 1-1
Statement of Task

The U.S. National Committee on Theoretical and Applied Mechanics (USNC/TAM) represents the United States in national and international activities related to the broad science of mechanics, including related sciences, engineering, and mathematics. It serves as a focal point for charting future priorities in mechanics related research, applications, and education.

An ad hoc committee will organize a national workshop in Fall 2015 to discuss the challenges and opportunities in theoretical and computational methods to advance additive manufacturing in a holistic, multifaceted, and interdisciplinary way. Experts from different sectors and industries will share their best practices and ideas to move the field forward.

The workshop will give researchers in industry, academia, and governmental sectors the opportunity to disseminate the fundamental knowledge that they have obtained related to additive manufacturing processes to contribute to the rapid scientific advancement of those processes. Workshop participants will also suggest short-, intermediate-, and long-term goals for a successful future in predictive methods for additive manufacturing applications. A rapporteur-authored summary of the workshop will be published, and a webinar provided.

the agenda. The workshop was held at the Keck Center of the National Academies in Washington, D.C., and was sponsored by the National Science Foundation, Sandia National Laboratories, and the National Institute of Standards and Technology.

Wing Kam Liu, serving as chair of the workshop planning committee, opened the workshop with a brief overview of the four focus areas:

1. Theoretical understanding of materials science and mechanics;
2. Computational and analytical methods in AM;
3. Monitoring and advanced diagnostics to enable AM fundamental understandings; and
4. Scalability, implementation, readiness, and transition.

The workshop was organized with three speakers per topic per day for the first two days. Each speaker was asked to identify the necessary short-, intermediate-, and long-term goals to advance predictive methods in AM as well as to address a set of predefined questions for each focus area. The third day of the workshop brought together speakers and attendees from each session to summarize lessons learned and identify unanswered questions.

Liu emphasized that this workshop would not focus on the policies needed to facilitate international collaboration among academic institutions, national laboratories, and industry. However, he noted that there are currently many stumbling blocks inhibiting collaboration, especially relating to intellectual property, and effective policies would be beneficial.

This workshop was organized under the guidance of the United States National Committee on Theoretical and Applied Mechanics (USNC/TAM), which represents the United States in national and international activities related to the broad science of mechanics, including related sciences, engineering, and mathematics. It serves as a focal point for charting future priorities in mechanics-related research, applications, and education and represents the United States in the International Union of Theoretical and Applied Mechanics (IUTAM). IUTAM represents 55 countries and 18 affiliated organizations.

Approximately 50 participants, including speakers, members of the planning committee, invited guests, and members of the public, participated in the 3-day workshop. The workshop was also webcast with nearly 200 online participants and 1,700 total video viewers.

This report has been prepared by the workshop rapporteur as a factual summary of what occurred at the workshop. The planning committee's role was limited to organizing and convening the workshop. The views contained in the report are those of individual workshop participants and do not necessarily represent the views of all workshop participants, the planning committee, or the National Academies of Sciences, Engineering, and Medicine.

In addition to the workshop summary provided here, materials related to the workshop can be found online at the website of the Board on International Scientific Organizations' U.S. National Committee for Theoretical and Applied Mechanics,[1] including the agenda, speaker presentations,

[1] The website for the U.S. National Committee for Theoretical and Applied Mathematics is http://sites.nationalacademies.org/pga/biso/IUTAM/, accessed August 23, 2016.

archived webcasts of the presentations and discussions, and other background materials.

ORGANIZATION OF THIS REPORT

Subsequent chapters of this report summarize the workshop presentations and discussions. Chapter 2 provides an overview of the theoretical understanding of materials science and mechanics, including related physical sciences, engineering, and mathematics, for AM. Chapter 3 focuses on computational and analytical methods in AM. Chapter 4 discusses monitoring and advanced diagnostics to enable fundamental understanding in AM. Chapter 5 provides an overview of scalability, implementation, readiness, and transition considerations for AM. Chapter 6 describes subgroup discussions regarding some of the recurring issues mentioned throughout the workshop as well as topics that need to be examined more closely. Lastly, Appendix A lists the workshop speakers, and Appendix B shows the workshop agenda.

2

Theoretical Understanding of Materials Science and Mechanics

The first session of the first two days of the workshop provided an overview of the theoretical understanding of materials sciences and mechanics applied to additive manufacturing (AM), including related physical sciences, engineering, and mathematics for AM. This includes but is not limited to design of metallic alloys or polymer blends, mixing and compatibilities of fundamental materials, heat source interaction with feedstock, heat source modeling, and incorporation of thermodynamic modeling into micro and macro heat transfer for the prediction of microstructures and metrology. Emphasis was placed on polymers, alloys, and alloy-polymer interfaces. Marianne Francois (Los Alamos National Laboratory), Peter Olmsted (Georgetown University), John Turner (Oak Ridge National Laboratory), Steve Daniewicz (Mississippi State University), Neil Hodge (Lawrence Livermore National Laboratory), and Saad Khairallah (Lawrence Livermore National Laboratory) each discussed research, challenges, and future directions relating to the following questions:

- What are the fundamental scientific issues of AM?
- What are the unique fundamental theoretical and computational approaches that need to be proposed and developed to fully understand AM?
- What are the mathematical models and state-of-the-art theoretical, computational simulation models that describe the different aspects of AM, and what new computational, statistical, and experimental

methods are needed to simulate the various stages of AM, going from feedstock mixture through deposition and consolidation, and ultimately assessing characteristics of the final product?

- What integration frameworks currently exist for coupling these modeling techniques together to advance AM?
- What are the most important open questions in materials and mechanics, including related scientific disciplines, engineering, and mathematics, as well as the technical challenges to be addressed for predictive theoretical and computational approaches in order to enable widespread adoption of AM?
- Does AM require unique fundamental research in theoretical and computational materials science, mechanics, and multiscale computation? What are the opportunities?
- What multidisciplinary and related materials and mechanical sciences are needed for AM?
- How will theoretical and computational models be verified and validated for AM processes?
- What opportunities exist for public-private partnerships to advance theoretical and computational mechanics capabilities for AM? How could these partnerships benefit from shared modeling and computation advancements?
- Do materials standards change with a theoretical and computations approach to materials development and implementation?

TOWARDS MODELING AND SIMULATIONS OF ADDITIVE MANUFACTURING OF METALS AT LOS ALAMOS NATIONAL LABORATORY

Marianne Francois, Los Alamos National Laboratory

Marianne Francois provided an overview of collaborative[1] efforts in modeling and simulation of AM at Los Alamos National Laboratory (LANL), which largely focus on metals and directed energy deposition processes. LANL's research in AM of metals is part of a multi-lab effort including researchers from Lawrence Livermore National Laboratory (LLNL),

[1] Francois recognized contributions from the following researchers: C. Bronkhorst, N. Carlson, C. Newman, V. Livescu, S. Vander Wiel, T. Haut, S. Runnels, J. Bakosi, J. Gibbs, J. Mayeur, A. Trainer, L. Parietti, D. Teter, J. Carpenter, G. Gray, T. Lienert, T. Holesinger, A. Clarke, D. Tourret, C. Knapp, J. Shlachter, M. Schraad, B. Archer, and K. Lam.

Sandia National Laboratory (SNL), and the National Security Campus (NSC). LANL's focus on directed energy deposition utilizes an electronic beam (e-beam) or laser beam as the heat source to melt the material, and powder or wire as feedstock.

She identified two key fundamental issues in AM: advancing science-based qualification of AM metals and shortening the qualification cycle to reduce cost. A lack of standards and certified processes for AM contributes to widespread variability. She commented that the multiple AM processes (e.g., powder bed, directed energy deposition), various operating conditions and control parameters (e.g., power, scanning patterns), varying feedstock quality, and different post-processing (e.g., heat treatment) can all impact the end product. Francois emphasized the need for fundamental understanding through a scientific methodology that integrates experiments with theoretical modeling and simulation.

The underlying material microstructures can dramatically impact material performance, as shown in Figure 2-1, Francois explained. In this figure, three microstructures of 316L stainless steel material are shown, where each varies due to processing differences (the material shown on the left was processed using AM, the middle was processed with the wrought method, and the right was processed using AM with a recrystallization heat treatment). In the material that was processed only with AM, different length scales for the microstructure can be seen. The wrought material, in contrast, has much smaller and more uniform grain size. The material with AM and recrystallization shows an even smaller microstructure. These different microstructures result in different damage profiles, as is also shown in Figure 2-1. Francois suggested that there should be a theoretical and computational approach to integrate processing and performance through microstructure prediction. She stated that advanced modeling and simulation capabilities for AM processes need to be developed, along with experimental testing, to advance methodology for prediction and control.

Francois outlined a long-term vision for microstructure-aware modeling, spanning and linking process modeling (e.g., a moving heat source), microstructure modeling (e.g., direct numerical simulation of grain growth), properties modeling (e.g., polycrystal models to determine elastic, plastic, and damage properties), and performance modeling (e.g., thermal-mechanical models to predict elastic, plastic, damage, and failure processes). Each of these AM modeling areas is being examined at LANL with the hope of better connecting them to design and then utilizing materials based on underlying parameters.

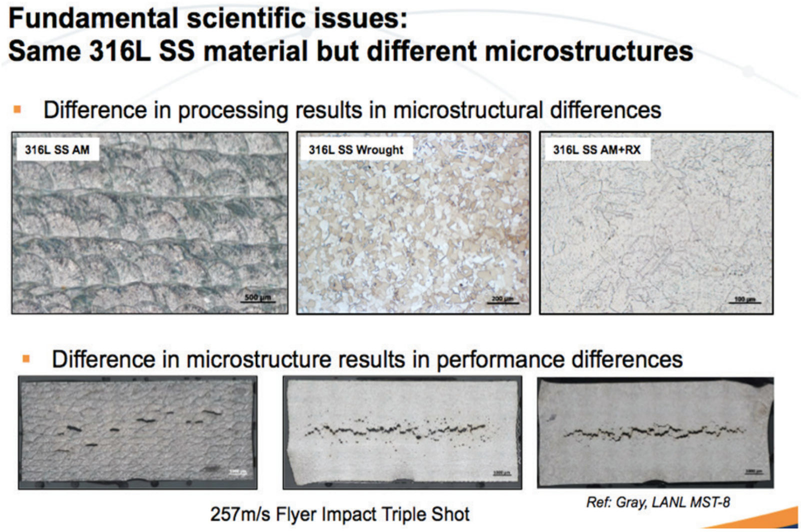

FIGURE 2-1 Material microstructure impact on performance. SOURCE: Marianne Francois, Los Alamos National Laboratory, presentation of Gray et al. (2015) to the workshop.

Francois reviewed specific examples of work being done at LANL. First, TRUCHAS,[2] a computational tool for modeling material processing, was discussed. This three-dimensional multiphysics package can model fluid flow with interface tracking and surface tension, heat transfer with phase change, species diffusion, and chemical reaction and solid mechanics. It also allows for complex geometries. TRUCHAS was initially developed by LANL to model casting processes but was extended to model laser spot welding in 2006. She described a validation study conducted on laser spot welding of 304 stainless steel (Parietti and Lam, 2006). This simulation starts with a solid piece of stainless steel and applies a heat source. As the material starts to melt, a melt pool region around the heat source develops. Temperature histories can then be plotted of a cross section and the top surface of the material to observe the behavior of the heating, the melting region, the phase-change region, and the resolidification over time. These results agreed with similar studies (He, Fuerschbach, and DebRoy, 2003).

[2] The website for TRUCHAS is https://github.com/truchas/truchas-release/, accessed August 15, 2016.

Francois explained that Marangoni convection determines the melt pool shape and it is important to predict its impact accurately. For example, it impacts the microstructure and determines where the grains of the weld beads are going to be located. The AM scanning pattern will result in weld beads overlapping, so understanding and controlling this pattern is important. She commented that surface tension is the main driver that determines convection in the melt pool. Specifically, if there is a negative gradient, there will be an outward flow that results in a shallower melt pool, and if there is a positive gradient, there will be in inward flow that results in a deeper melt pool. Surface tension properties can vary with material composition and temperature, and impurities will change the melt pool shape and size, Francois explained. She highlighted several topics in AM that currently need more research, including the effects of fully- or partially-melted powder particles being added to the melt pool, the effects of the scanning pattern on the melting and resolidification cycle, and the role of chemical composition and surface instabilities on final results.

Currently, Francois explained, TRUCHAS is being extended to model directed energy deposition AM processes. The capabilities are being assessed via testing on AM process problems involving heat transfer and phase change, melt pool fluid flow (Marangoni effect), and residual stress and distortion. The research at LANL in this area is currently focused on implementing preliminary heat and mass deposition models with moving heat flux boundary conditions for simpler models, and fully moving powder and laser energy deposition at evolving material surface embedded within the computational domain. In the future, they plan to explore more physics models and verification and validation, as well as to develop microstructure-aware solidification models.

Microstructure evolution is being studied at LANL—specifically, grain growth evolution during solidification on flat and curved surfaces—using an implicit phase field approach to microstructure solidification simulation utilizing modern algorithms and software. She noted that most current phase field models utilize explicit methods that are time consuming because they require small time steps. In contrast, implicit time integration allows for stable solutions to be developed with large time steps, therefore completing the analysis more quickly. Francois also added that finite element approaches allow for high-order spatial discretization on unstructured two- and three-dimensional meshes, and unstructured mesh allows for irregular geometries. Some verification test cases for single grain growth in two and three dimensions have been conducted to compare accuracy.

Francois emphasized that predicting macrostructure performance will require better microstructural representation. Performance and properties modeling of AM materials are being examined, specifically with respect to damage, metallographic characterization, and strength. She commented that the influence of microstructure is significant, and it is not yet possible to represent the AM adequately to successfully predict dynamic damage with simple macroscale models. Metallographic characterization is done by extracting microstructure data from experiments and by utilizing Dream.3D[3] software to generate the microstructure digitally, Patran[4] finite element software with advanced surface meshers to model the polycrystalline microstructure, and Abaqus[5] finite element damage model to evaluate the microscale. Strength differences between wrought stainless steel and AM with recrystallization showed that the AM-processed materials have a smaller mean grain size, which generally increases strength in materials. Francois explained that researchers are currently studying whether the grain size difference is in part responsible for an observed strength difference between these manufacturing processes.

She concluded with a discussion of the long-term objectives and future opportunities for predictive methods in AM as listed below.

Long-term objectives for theoretical and computational predictive methods in AM:

- Integration of processing and performance modeling through microstructure prediction;
- Validation with experimental testing (in situ) as part of the methodology towards prediction and control;
- Development of multiscale process modeling that is microstructure-aware; and
- Expansion of AM materials modeling and multiscale mechanical response (performance) modeling—e.g., processing phase change and microstructural evolution, cooling internal stress development linked to microstructure, and plasticity and structural feature damage prediction.

[3] The website for Dream.3D software is http://dream3d.bluequartz.net/, accessed August 15, 2016.

[4] The website for Patran is http://www.mscsoftware.com/product/patran, accessed August 15, 2016.

[5] The website for Abaqus is http://www.3ds.com/products-services/simulia/products/abaqus/, accessed August 15, 2016.

Future opportunities for theoretical and computational predictive methods in AM:

- Material processing
  - —Melting and solidification cycles, melt pools, microstructure morphology evolution, alloy composition distribution, liquid-solid phase change models;
  - —Linkage of microstructure information to macroscale model (e.g., thermal gradient and cooling rate maps); and
  - —Residual stresses.
- Mechanics of materials
  - —AM materials models and properties (e.g., solid-solid phase transformation);
  - —Plasticity and damage modeling; and
  - —Linkage of microstructure information to macroscale model.
- Faster computational methods
  - —Reduced-order models, fast emulators for process control; and
  - —Robust, efficient, and accurate numerical methods for high-fidelity physics-based simulation (e.g., implicit methods).

CHALLENGES IN ADDITIVE MANUFACTURING OF SOFT MATERIALS: POLYMER-BASED FUSED DEPOSITION MODELING

Peter Olmsted, Georgetown University

AM for soft materials is currently being examined through a joint project between researchers at Georgetown University[6] and the National Institute of Standards and Technology (NIST),[7] Peter Olmsted explained. This project includes polymer-based fused deposition modeling, selective lithography, and laser sintering; the first of which was the focus of his presentation. He explained that many issues can arise with AM, such as poor material fibers adherence, weak mechanical properties, sagging, poor or textured surface properties due to sub-millimeter sized threads, undesired porosity, shrinkage, warping, and debonding. Materials properties, he emphasized, need to be better understood to move use cases for polymer AM beyond prototypes.

Olmsted provided a brief overview of the scientific areas and the challenges of fused deposition modeling of polymers (P-FDM). Fused

[6] Peter Olmsted and Claire McIlroy.

[7] K. Migler, J. Seppala, A. Kotula, R. Sheridan, G. Gillen, A. Forster, J. Bennett, J. Kilgore, and R. Ricker.

deposition modeling is sometimes known as "hot glue gun" extrusion because the process starts with a reel of solid filament, which then gets melted and extruded to lay down the material, as shown in Figure 2-2. The properties of laying down the material are non-isothermal and have not been sufficiently addressed in the polymer modeling community. He also described the challenge of balancing the need for rapid prototyping with the need for parts to be sufficiently strong with desired characteristics. Molten polymers, he noted, can either be glassy (amorphous)[8] or semi-crystalline,[9] and these differences pose distinct challenges with processing and mechanical properties.

Physical properties often need to be examined to better understand how to process materials. In the case of crystalline materials, when the polymer is extruded out of the nozzle, it leaves an oriented polymer filament that is more likely to crystallize. Therefore, the crystalline morphology reflects the properties of the processing and impacts the mechanical properties. Olmsted explained that ideally filaments would be entangled with each other to increase bonding between layers. Polymer rheology can also give rise to non-Newtonian fluid phenomena, such as shear thinning, rod climbing, die swell, and spurt and slip. He emphasized that many molecular features are not yet captured in modeling. Notable issues in P-FDM discussed by Olmsted include crystallization and glass transition and their potential to better inform polymer welding.

Crystal nucleation during extrusion from contraction flow can occur (Scelsi et al., 2009; Doufas, McHugh, and Miller, 2000; Doufas et al., 2000; Graham and Olmsted, 2009). To optimize crystalline materials, measurements of crystallinity need to be linked both in situ and ex situ with the modeling of the development of the crystallinity as well the effect of the crystallinity on the mechanical properties.

Glassy or amorphous polymers do not undergo the large structural change of semi-crystalline polymers, so a more amorphous isotropic material can be developed. But, he cautioned, researchers need to be thoughtful about the behavior around the glass transition. While the understanding of glass transition in polymer glasses is evolving (Forrest and Ediger, 2014; Angell, 1997), Olmsted stated that additional research is still needed. He explained that this area is particularly important to understand because

[8] Examples of glassy molten polymers include polycarbonate (PC) and acrylonitrile-butadiene-styrene (ABS).

[9] Examples of semi-crystalline molten polymers include poly-caprolactate (PCL) and polylactic acid (PLA).

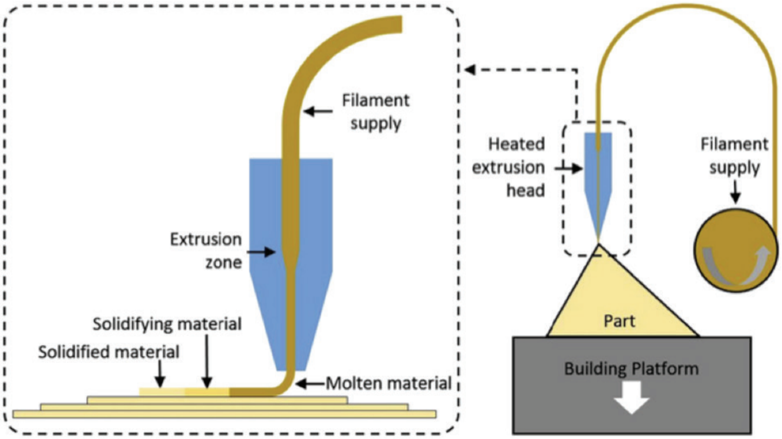

FIGURE 2-2 Fused deposition modeling process. SOURCE: Peter Olmsted, Georgetown University, presentation of Bikas et al. (2016) to the workshop.

there is increased mobility in the surface layer (top 10 to 20 nm) of polymers as the glass transition is approached. When a filament is extruded, it cools to below the glass transition point as it solidifies. However, it would be better if the previous filament is reheated above the glass transition point as the next filament layer is extruded to form a weld between the layers (Ge et al., 2013; Ge, Grest, and Robbins, 2014). He emphasized that if the weld properties between the filaments could be improved, the overall material properties would improve.

There are also computational modeling challenges that need to be addressed, according to Olmsted. Many time-dependent quantities need to be coupled in a multiphysics type of approach. In particular, understanding the molecular shape, structure, orientation, and alignment through the filament at the center and the edges is essential to understanding the flow through the filament. This needs to be coupled to the changing temperature field, the non-Newtonian fluid mechanics, the density changes, the moving and changing boundaries between solid surfaces and free surfaces, and, if crystallinity is involved, the effects of phase change materials on latent heat and time scales. These span multiple scales from the microscale to the continuum. For example, he stated that continuum modeling of non-isothermal processes such as fiber modeling includes the following parameters: momentum, conformation, stress constitutive relation, heat flow, crystallinity, and time (Doufas, McHugh, and Miller, 2000).

Polymer processing was discussed as an example where assembling a large research team to work across scales was successful. With the goal of manufacturing films at large industrial scales, researchers used reaction chemistry to inform molecular shape, which fed into constitutive modeling to help define the macroscopic properties of the melt. These results were then compared with experimental results. Several universities (Leeds, Cambridge, Durham, Bradford, Sheffield, Oxford, and Eindhoven) and industry partners (e.g., BASF, Innovene, Mitsubishi, Dow, DSM, ICI, and Lucite) formed a consortium to study the polymer rheology, flow-induced crystallization, instabilities, design-for-process, materials, and product properties. This consortium worked for over 10 years to connect theory, chemistry, experiments, and industrial materials. He suspects a similar effort for AM would be needed.

Olmsted noted the work of the Materials Genome Initiative (MGI) at NIST, which aims to develop a predictive materials database for AM; to predict mechanical properties, prototype speed, resolution, and processing parameters based on polymeric properties; to develop a seamless link between advanced metrologies, computation and prediction, and materials properties; and to shorten times for development of new protocols and products.

Olmsted emphasized that there is a need for new in situ metrologies to go along with model development. Necessary measurements include temperature, molecular conformation and shape, welding and interfacial properties, mechanical properties (e.g., elastic moduli, fracture strength and toughness, anisotropy, and plasticity), and crystallinity. Spectroscopies (e.g., infrared, X-ray, neutron, Raman, and fluorescence), microscopies (e.g., light, Raman, transmission electron, and scanning electron), and interfacial characterization (e.g., neutron scattering) could all be used to advance measurements.

In conclusion, Olmsted summarized the theory and computational needs for P-FDM at different scales. At the micron scale, coupled molecular and thermodynamic fields (e.g., temperature, mass, velocity, crystallinity, and orientation) need to be developed. At the nanometer scale, polymeric atomistic (or united atom model) simulations to model welding and deformation of materials are needed. On the millimeter scale, finite element simulations of parts and pieces should be developed and compared with experimental results on deformation, fracture, and yield. Experimental inputs and metrologies (e.g., temperature, extrusion conditions, build protocols) should be used for material models. Theory and prediction should be built around model materials as well as "wild" materials.

Lastly, he highlighted some of the main questions remaining in P-FDM:

- *Fundamental scientific issues* include how to handle non-isothermal conditions, molecular alignment, and welding, as well as how to understand how phase changes (e.g., crystallization and the glass transition) impact production, especially when shrinkage and warping occur.
- *Unique fundamental theory and computational approaches* include spanning multiple scales (molecular [nm] to part size [cm]), connecting multiple dynamic fields (e.g., temperature, velocity, deformation), and solving complex molecular and non-linear rheology and constitutive relations.
- *Mathematical models and validation* of relevant materials models include the rheology of advanced models for polymer deformation, including both computation (e.g., flow solvers for complex non-isothermal constitutive models for different build protocols) and experimental (e.g., in situ characterization of temperature and orientation; weld properties and mechanical performance) results.
- *Open questions in materials and mechanics* include the glass transition, flow-induced crystallization, and the relation of polymer molecular structure to fracture strength and deformation.
- *Unique fundamental research for AM* includes the glass transition, polymer dynamics, interfaces, and other areas.
- *Multidisciplinary sciences are needed*, including mathematics, computation, engineering (e.g., chemical and mechanical), metrology, physics, and chemistry.
- *Research partnerships* would advance the community, especially those that bring together national laboratories (e.g., NIST) and industry (e.g., polymer manufacturers, AM equipment and process developers, and AM users).

MODELING AND SIMULATIONS OF ADDITIVE MANUFACTURING

John Turner, Oak Ridge National Laboratory

Turner began by giving an application example comparing a projectile hitting a block of titanium (Ti) to armor created by sandwiching a titanium diboride (TiB_2) center with two Ti plates. The three-dimensional Ti plates were created using AM and were designed to have varying angles on the inner-facing side of the plates. The TiB_2, which is an extremely hard ceramic, was then injected into the cavity between the two Ti plates. Ultimately, this new configuration with TiB_2 provided better protection with a lower weight than the Ti alone.

He explained there are two types of AM technologies that can be used to create a system such as this: (1) large melt pool technologies, including plasma, e-beam, and laser using wire feedstock; and (2) powder-bed technologies, including laser and e-beam using powder feedstock. While these technologies have differences in their particular methodologies and characteristics, their underlying physical processes are similar. This is especially true for energy deposition, melting and powder addition, evaporation and condensation, heat and mass transfer, solidification, solid-state phase transformation, repeated heating and cooling, and complex geometries. Because of these similarities, many aspects of the models used to simulate these processes can be applied to different fusion technologies. Also, these models are complex coupled multiscale physics processes that span the microstructure (e.g., grain size), the powder properties, the mesoscale, and the engineering scale. Turner noted that there are both numerical and software challenges to building these applications:

- *Computational times.* The build times of these large and complex simulations can take hours and brute force approaches will not work.
- *Large temperature gradients.* Large temperature gradients and rapid heating and cooling require coupling between thermomechanics and the melt and solidification processes.
- *Heterogeneous and multiscale simulations and parameters.* The resolution of energy sources and effective properties of powder for continuum-scale simulations can be challenging.
- *Path optimization.* The optimal path for the energy source for complex parts needs to be determined.
- *Large number of parameters and missing understanding.* Key uncertainties in feedstock properties and process parameters can propagate through the simulation.

- *Validation.* Validation is difficult as characterization is limited. Turner said that national laboratories could have a role to play in improving validation through unique experimental facilities.[10]

A broad spectrum of computational science is required to fully realize the promise of AM, Turner emphasized. The physics of the AM process (e.g., energy interaction with porous materials, gas-liquid-solid reactions, rapid melting, solidification and crystallography, elastic and plastic strain, and evolution solid-solid phase transformation under thermomechanical cycling) and applied mathematics and computer science (e.g., coupled large-scale partial differential equations, multiscale coupled physics, uncertainty quantification and design under uncertainty, risk analysis and decision making, scalable software, large-scale inverse problems, and large-scale optimization) need to work in tandem with characterization, experimental validation, and high-performance computing infrastructure. In some cases, Turner commented, models, techniques, and capabilities in these areas exist for other applications and can be brought to bear on challenges of AM. He also noted that computational capability has increased at a relatively steady pace for decades, making significant advances in this field possible.

Turner then discussed scale-specific challenges, including that of the powder (e.g., properties and melting), the mesoscale, and the engineering scale (e.g., the relationship between process parameters and microstructure). The selective laser melting process is sensitive to particle-level variations. Areas of exploration include measuring heat transfer in powders and packed beds and developing simulations to get effective properties such as conductivity, laser penetration and distribution, melting, and solidification.

Turner then offered some examples of current research being conducted in this area. Particle melt modeling, for example, is approached first by developing a relation for powder-bed melt percentage as a function of laser power added. The powder bed is represented as spherical particles superimposed on a background mesh. Then, the discrete element model with the multiphase code MFiX[11] can be used to model particles melting and shrinking due to applied heat source.

Phase field simulations are used to understand microstructural evolution. These models have several notable features. They can be fully

[10] One example an experimental facility that could provide value is the Spallation Neutron Source at Oak Ridge National Laboratory (ORNL).

[11] The website for the National Energy Technology Laboratory's software suite is https://mfix.netl.doe.gov/, accessed August 15, 2016.

integrated with system thermodynamics, and the system energy includes contributions from anisotropic interfacial energy and elastic energy due to transformation strains. The governing equations of the model are solved using the Fourier spectral method, often using large runs with thousands of processors. There is also a unique composite nucleation model that allows growth of specific variants assisted by local strain field. Turner explained that phase field simulations indicate that the nucleation rate is the main factor responsible for the formation of colony structure. Furthermore, low nucleation rate promotes colony formation when a new nucleus sees well-developed strain field from a nearby variant. High nucleation rate promotes basket weave formation when all nuclei experience a complex strain field.

Turner then gave an overview of a recent project using electron beam AM. The process begins with a three-dimensional CAD model, which is discretized into two-dimensional layers. The part is then created by adding successive layers, typically using a back-and-forth raster melt sequence known as an oxen path. Research was performed to determine if spot melting could be used to better control this process. Although microstructure manipulation via AM is not yet fully understood, it typically results in columnar grains oriented along the build direction. To study if this behavior could be controlled, researchers have adapted TRUCHAS (the LANL code developed to model metal casting processes and previously discussed by Marianne Francois) for AM applications. Specifically, TRUCHAS is used to approximate the thermal gradient at the liquid solid interface (G) and the velocity or growth rate (R) of liquid-solid interface, both of which are difficult to measure experimentally, and also to examine the significance of other process parameters (Dehoff et al., 2015; Lee et al., 2014). By adjusting process parameters, the G and R values for the melt pool can be specified such that the grain structure (equiaxed vs. columnar) can be locally controlled (Raghavan et al., 2016).

Turner summarized that this research relies on multiple physics (e.g., conduction, convection, thermal radiation, solid-solid phase transformations, melting and solidification, fluid flow with surface tension, and solid mechanics) and numerical approaches (e.g., particle methods, view factor radiation, discrete element methods, phase field methods, finite volume methods, and finite element methods). He emphasized that tools exist that provide some combination of these capabilities, but few, if any, provide all the capabilities needed to study AM processes.

Lastly, Turner summarized four key ideas from his presentation: (1) Physical processes during fusion-based AM have much in common with other manufacturing processes like casting and welding, including heat and mass transfer, melt and solidification, solid-state transformation, distortion, and residual stress; (2) Efforts are underway to repurpose existing tools and develop new tools for analysis and control of powder properties and behavior; (3) Solid-state microstructure evolution can also be predicted by coupling overall transformation kinetics and thermal cycles; and (4) Control of solidification structure can be achieved by controlling temperature gradient and liquid-solid-interface velocity within the melt pool.

Discussion

Following their presentations, Marianne Francois, Peter Olmsted, and John Turner all participated in a panel discussion moderated by the workshop chair Wing Kam Liu from Northwestern University. The first question was posed by a virtual participant regarding how the different modeling stages are linked, given that there can be a strong interaction between these stages in relation to the material modeling. Francois explained that it started with molecular dynamics simulations, process modeling, microstructure modeling, and properties modeling. Linking these models is an open research question, and she said the community is open to suggestions and collaborations. On the processing side, she mentioned the relevance of John Turner's work to bring information from the continuum scale model of the processing, accounting for the topological gradient and velocity of the phase change, to better understand the corresponding microstructure.

Another participant commented that many material, physical, and thermal properties have been identified as critical to study as well as flow momentum, deformation, phase change, and orientation. Considering that modeling with these phenomenological understandings is the next phase, the participant asked how to prioritize research on the phenomena as well as which phenomena have the most challenges to measure or understand. Olmsted noted that in polymeric fused deposition modeling, the orientation of the polymer material is extremely important and is easy to measure if there is a homogeneous degree of orientation. However, fused deposition modeling of filaments has a thin skin layer whose orientation is crucial to understanding how well the material bonds. Information about this skin layer orientation needs to be properly extracted experimentally, and the modeling needs to be able to capture the inhomogeneity to understand the molecular properties at the weld between the two materials. There are challenges facing the metrology and the modeling of the interface. The latter can be done at an atomistic simulation level and then brought up to a coarse grain model to understand the mechanics of a more heterogeneous material. Turner commented that the physics of solidification and melting are important to understand. This includes factors such as the interaction between the powders and the energy beam on the energy deposition. He cautioned that the surface finish is very important but is difficult to simulate and control. Francois stated that it is important to keep in mind the desired final product. Building stronger materials requires microstructure control, including the process parameters. If the goal is a product with a polished surface, machining after directed energy deposition is likely necessary. The process used, including the process parameters and the build geometry, depends on what type of product is desired, and thought needs to be given as to how to certify the part.

A remote participant wondered if it is practicable for the federal agencies to set up schemes for sharing data, thereby enabling data mining and data analytics. The participant asked if this would be fair to the originators of such data, especially when a large effort is required such as from synchrotron research. Turner responded that national laboratories would like to advance information sharing and have made attempts toward it in the past. While there are proprietary restrictions on data and geometries, he believes it would benefit the community to have common test problems and property data that can be used and shared.

An audience member asked about the practical significance of the transition from columnar grain growth to equiaxed as well as if the motivation is to avoid anisotropy. Turner responded that the columnar and equiaxed grain growth have different final strength properties. The ability to control which structure exists in different parts of a material would be a significant advance.

A participant from a national laboratory asked about the complexities and challenges of repurposing codes for AM. Turner referred to his and Francois's discussion of the open-source TRUCHAS code, which was designed for casting, not for adding material. He explained that the software had to be significantly adapted and continues to evolve; however, the effort required for this transformation is often underappreciated. Francois agreed, noting that the underlying physics modeled (e.g., heat transfer with phase change, fluid flow) are similar but the differences (e.g., mass and energy deposition) can require significant work. There are still AM-specific modifications and capabilities that need to be decided upon and developed. In addition, the revised code also needs further refinement, verification, and testing. Turner elaborated that there are challenges with the physics, numerical approaches, and software that need to be addressed. For example, he described an analysis where the output was needed to conduct the necessary processing and mapping. Connecting these tools and steps more seamlessly would be helpful.

A participant referenced the discussion about microstructure entanglement and the different impacts of cooling rate. He asked how cooling rates could be controlled in AM processes to achieve the desired microstructure. Olmsted emphasized that this is challenge. He and collaborators at NIST have been able to measure the temperature profiles as a function of time, and the next step is developing strategies to control the cooling rate. Ideally, the welding would occur in a warm region between the filaments while the rest of the filaments are stable and the part is structurally sound. The goal is to work at the interface to enable effective mobility and heat transfer while maintaining the mechanical properties of the part.

An online participant commented that the microstructure of the deposited alloys also contains impurities. He asked how the formation of these defects can be predicted and how their effects on the macroscopic mechanical properties can be simulated. Turner responded that handling defects is challenging, and their work so far is focused on pure or ideal materials and well-defined mixtures. However, he suspects that phase field modeling with randomly introduced nucleation points could be applied to defect modeling.

An online academic participant asked if samples could be obtained from ORNL or Sandia for experimental analyses. Turner said this is possible and there are a number of programs to facilitate this, including their manufacturing demonstration facility that works with companies of all sizes. In conclusion, Liu emphasized that clarifying these processes would help encourage university-industry-government partnerships.

THEORETICAL UNDERSTANDING OF MATERIALS SCIENCE AND MECHANICS

Steve Daniewicz, Mississippi State University

Steve Daniewicz explained that his presentation would focus on two of the overarching session questions: What multidisciplinary and related materials and mechanical sciences are needed for AM? And, do materials standards change with a theoretical and computational approach to materials development and implementation? His emphasis was on metals, in contrast to the preceding polymer-focused discussions described in this chapter.

The AM process is complex, he explained, and can be illustrated as shown in Figure 2-3. Some of these technologies have been around for decades through fusion welding and can be built upon for AM. In contrast to the fusion process, there are two unique components of the AM process: the interaction of the power source and the powders, and the thermal history (e.g., welding at high velocities, melt pool solidification, and solid-state phase transformations occurring at higher rates). He explained that the unique thermal histories result in unique microstructures. Porosity, mechanical failure, residual stress and corresponding distortion, and fatigue are issues to be considered. There are several multidisciplinary scientific needs, as described by Daniewicz:

- Powder-heat source interactions,
- Microstructure evolution under non-equilibrium conditions,
- Heat transfer in melt pool and heat-affected zone,
- Origins of metallographic texture,
- Elastic-plastic constitutive relationships,
- Residual stress and distortion prediction,
- Melt pool solidification, and
- Physics of porosity development.

He emphasized that better understanding of the microstructure evolution is key to approaching many of these challenges. This understanding includes the process parameters (e.g., material, tool path, laser, scan speed), the heat transfer (e.g., cooling rate, thermal history, thermal cycling), the microstructure, and the mechanical properties, all of which are connected. With respect to the heat treatment, Daniewicz gave the example of Ti-6Al-4V manufactured four ways—as-built, annealed below β-transus temperature,[12] heat treated above β-transus temperature, and wrought—and showed that the microstructure and fatigue life are impacted. In particular, there was a reduction of fatigue life of AM Ti-6Al-4V in contrast to the wrought product (Sterling et al., 2015) from a strain-life perspective. He commented that there is a higher monotonic strength (both ultimate and

[12] The lowest temperature at which a 100 percent beta phase can exist is called the beta transus; this can range from 700°C (1,300°F) to as high as 1,050°C (1,900°F), depending on alloy composition.

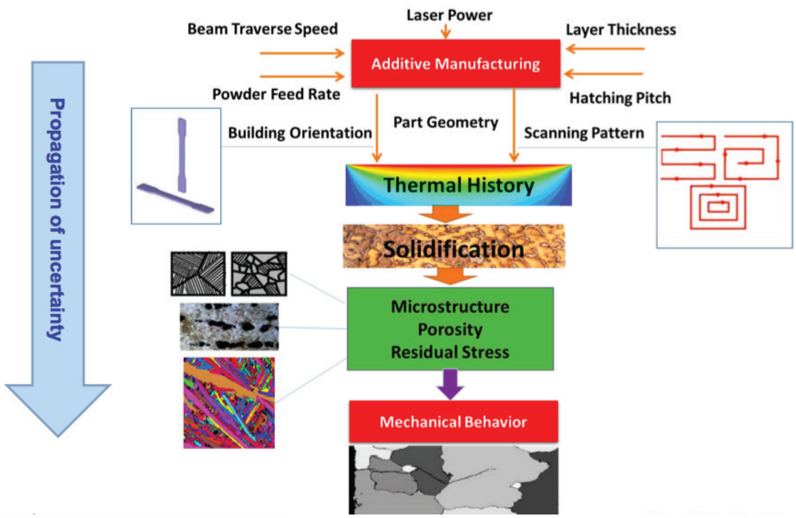

FIGURE 2-3 Additive manufacturing process. SOURCE: Steve Daniewicz, Mississippi State University, presentation to the workshop.

yield strength) and less ductility for AM direct laser deposition Ti-6Al-4V as compared to the wrought version. There is anisotropy as well, with different strengths resulting from a vertical build versus a horizontal build. He stated that one approach to make additive parts more like wrought parts is to use a hot isostatic press (HIP) as a post-build treatment to reduce anisotropy and improve fracture toughness (Kobryn and Semiatin, 2001). Residual stress is also an important consideration and one that has been studied in conventional parts for several decades (Masubuchi, 1980), according to Daniewicz. Understanding how thermal gradients produce residual stresses and subsequent distortion in additive parts is an ongoing research area.

The choice of whether or not to apply the HIP treatment to an additively-built part can either bring the material back to the properties of the wrought or take advantage of additional strength with uncertainty as to how the part will respond to distortion, respectively. He emphasized that distortion properties can be crucial, especially when parts need to be machined.

The unique additive microstructures have the potential to be exploited to tailor materials for specific applications. However, Daniewicz stated that this is a complex, multiphysics problem and many of these advances depend on high-performance computing to quantify the service environment and potential loading, use a microstructurally-aware mechanical model to predict part performance virtually, optimize microstructure and determine a target thermal history, and determine process and design parameters to produce parts via additive manufacturing.

Mechanical and materials science key issues in the short, intermediate, and long term were discussed by Daniewicz. In the short term, he said better understandings of nonlinear elastic-plastic constitutive relationships, material properties at elevated temperatures, and residual stress and distortion are needed. For the intermediate term, research in microstructure evolution under non-equilibrium conditions would be helpful. The long-term goal is to use thermal monitoring and control to optimize builds and exploit unique microstructure.

There is a strong need for standards to help understand variability, uncertainty, and reproducibility issues, Daniewicz emphasized. The standards organization ASTM International[13] has several working groups[14] aimed at improving AM standards. However, existing standards are in their infancy and need to be advanced in a number of areas, including generalized standards relating to terminology, processes and materials, test methods, design and data formats, and specialized AM standards relating to raw materials, process and equipment, and finished parts. These and their subcategories are shown in Figure 2-4. He emphasized that the current lack of process and testing standardization causes variability in results. An intermediate-term goal is to better understand the differences between coupons and components. In the long term, virtual prototyping can accelerate standards development and lessen variability.

PART-LEVEL FINITE ELEMENT SIMULATION OF SELECTIVE LASER MELTING

Neil Hodge, Lawrence Livermore National Laboratory

Neil Hodge began by stating that there is great potential for selective laser melting (SLM) AM, but many significant challenges exist. In particular, part-scale modeling is needed to inform part-specific configurations and

[13] The website for ASTM International is http://www.astm.org/, accessed August 15, 2016.

[14] Specifically, ASTM committees F42 on additive manufacturing, E08 on fatigue and fracture, and E07 on nondestructive testing.

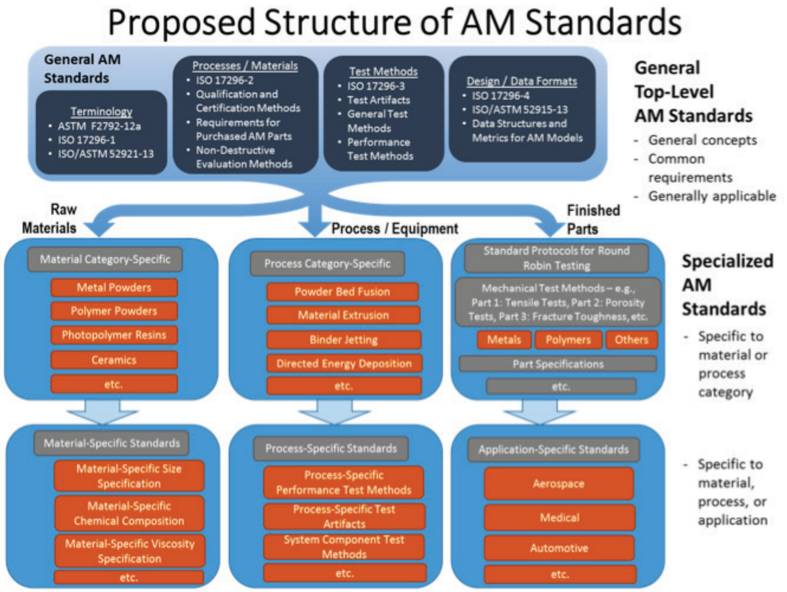

FIGURE 2-4 Proposed structure of additive manufacturing standards. SOURCE: Steve Daniewicz, Mississippi State University, presentation to the workshop.

processes. When he and his colleagues[15] at Lawrence Livermore National Laboratory (LLNL) started trying to develop models for SLM, they began with LLNL's Diablo code, which is a highly parallelized, implicit finite element code that can solve classical balance laws for solid mechanics (e.g., balance of thermal energy, balance of linear momentum) and associated thermal moving boundary problems. Diablo is now being extended to model the following features of SLM: successive activation of mesh regions, general laser path input definition, solid-only representation, powder as a low-strength solid, powder-to-solid as an irreversible phase transformation, and rule of mixtures response in partially transformed elements. Researchers started with simple modeling abstractions, such as how to represent the powder and how to handle geometric issues, and noted that the code required substantial changes to work for SLM.

A significant driver for SLM problems is the heat source. Hodge and his collaborators adopted an existing energy deposition model based on an

[15] Collaborators include R. Ferencz and J. Solberg in the Methods Development Group and R. Vignes in the Computational Engineering Division.

analytical solution to a radiation transport equation for a laser impinging on a powder (Gusarov et al., 2009), which seems to work well for SLM. They then turned to modeling single-track experiments, which required additional physics, including evaporation (where an analytical expression was developed to define a Neumann boundary condition) and recoil (represented as a phenomenological constitutive relation, implemented via anisotropic thermal conductivity). A participant asked Hodge where the residual stresses came from in the Diablo simulation. Hodge responded that the thermal gradients are the largest contributor to the residual stresses.

Using this code, Hodge and his collaborators were able to examine other characteristics of SLM, including the complex thermal evolution. This study demonstrated that temperature histories can feed microstructure predictions, and cooling rates were higher than expected. Also examined were overhangs, which are formed when lateral perforations require fusing above unprocessed powder to form downward-facing surfaces. These impact dimensional fidelity and surface finish, and re-machining the internal passages is often impossible or undesirable. Hodge and colleagues were able to represent a 0.5 mm overhang with constant laser powder and achieve results comparable to experimental results. Modeling and simulation can help identify mitigation strategies, Hodge noted, so they developed an overhang mitigation simulation that scaled down the laser power linearly once the laser was traversing onto overhang territory. Doing this, they were able to reduce the unnecessary thickness developing over the overhang. Once the overhang was sufficiently established, laser power could be ramped back up to full strength without distorting the part geometry.

Part-scale modeling creates additional challenges in moving from mm^3 to at least cm^3 scale, particularly in determining the time scale of global heat transfer and exploring further modeling abstractions (e.g., aggregated layers and scans). Hodge and his collaborators first attempted this using a prism specimen with a vertical build, original layers aggregated as 1 mm "superlayers," and coarse laser scanning. This model ignored powder outside the volume of the part. When comparing these modeling results with experiments (Wu et al., 2014), Hodge noted that the results are encouraging but show sensitivities. Hodge emphasized that stress evolution is nontrivial, even for simple geometries, and neutron diffraction data is another source of experimental comparison. Hodge highlighted some areas of future work relating to physics and process:

- Materials (e.g., general thermal-inelasticity, determination and representation of multiple solid states, integration with mesoscale models);
- Fracture;
- Laser path and power (e.g., integration with machine control algorithms and software);
- Support structures (e.g., continuum, structural, or both; integration with support structure generation packages); and
- Representation of build chamber, baseplate, and machine influence.

Simulation time is an obstacle, Hodge said, and cm^3 models can take on the order of hundreds of hours due to their nonlinear physics and significant ratio of length scales. One option to shorten the run time is to decouple the different length scales. He commented that initial testing indicates significant decreases in runtime versus the analogous, globally-refined mesh. However, work remains to get the desired performance and workflow. Other options may be to further explore physics-dependent time integration (e.g., time stepping), physics- and spatially-dependent dynamics, improvement of the phase change algorithm, discretization methods to handle geometry and multiple scales including contact (e.g., between part and baseplate) and higher order elements (e.g., polynomials and splines), and integration with geometry definition (e.g., primary solid model generation and slicing packages).

Hodge concluded by summarizing that SLM modeling and computational strategies to date are promising, particularly with distortions and stresses. He noted that there is a need for improved material representations, while simultaneously increasing computation speed, and that the data flows within the code federation should be formalized. Lastly, there are many opportunities to partner for user workflow utilities, from design geometry to SLM machine instructions.

MAIN PHYSICAL PHENOMENA IN METAL POWDER-BED FUSION

Saad Khairallah, Lawrence Livermore National Laboratory

Saad Khairallah began by proposing that the main challenge in AM is selecting the correct process parameters for a final product that meets engineering standards. He explained that the SLM process is complex and defects can be easily introduced. For example, defects at the single powder layer may lead to more defects in subsequent layers, including pores, incomplete melting, rough surface, bad wetting, low density, and poor overall quality. He stated that the understanding of the interplay between process parameters (e.g., laser power and speed, powder distribution and thickness) is still lacking.

To enhance this understanding, Khairallah and his collaborators developed a mesoscopic three-dimensional simulation of metal powder-bed fusion using the LLNL code ALE3D.[16] He showed simulation results of a laser traversing a stainless steel powder bed, with a strong melt flow and indications of incomplete melting. From this simulation, he framed his presentation into three key areas:

1. Physics: What are the driving physics?
2. Pore generation: How do pores form and evolve?
3. Suggestions: What is the guidance for better parameter choice?

The strong hydrodynamical effects under the laser include indentation that digs deep into the substrate, creating a backward melt flow and a vortex that follows the indentation. These effects are due to the recoil force under the laser from evaporation, surface tension (Marangoni effect), and cooling via evaporation and radiation. Khairallah elaborated that the maximum temperature below the laser results in boiling and evaporation. The particles then leave the surface with high kinetic energy and, in doing so, take energy away from the melt and help cool it. At the same time, the particles impart a recoil momentum on the melt that results in a topological deformation. Khairallah was asked by a participant if mass loss is accounted for in the evaporation rate. He responded that the mass loss is not significant and is not simulated; the strong recoil effect associated with evaporation is the dominant force. The surface tension that depends on temperature results in the Marangoni effect, which creates a strong melt flow.

In the process of starting from a solid powder, melting, and solidifying to a solid track, Khairallah explained that the laser creates an indentation that forms a pore upon collapse. The spillover helps create a denudation zone. The lateral asymmetrical melt flow and backward flow increase track volume. However, side pores are generated by denudation and strong lateral

[16] To read more about ALE3D (Arbitrary Lagrangian-Eulerian 3D and 2D Multi-Physics Code), see https://wci.llnl.gov/simulation/computer-codes/ale3d, accessed August 29, 2016.

melt flow. He explained that overlapping scan vectors at 75 percent can mitigate the side pores and the incomplete melting at the denudation zone. Also, a gradual laser ramp down prevents the formation of end-of-track pores.

The recoil and surface tension are the main driving forces, he explained. Recoil pressure dominates at high temperature with an exponential dependence on temperature, and surface tension dominates at lower temperatures. This means that recoil pressure dominates around the laser indentation and surface tension dominates at the track transition and tail end. Cooling limits the peak melt pool temperature and the recoil effects. Radiation cooling due to the Stefan-Boltzman Law (i.e., black body radiation) is not a huge force, Khairallah noted. Evaporative cooling has the largest impact because it is more efficient at high temperature due to exponential dependence on temperature. Marangoni cooling also plays a role because the temperature gradients create a backward flow and help disperse heat away from indentation. He explained that the melt track breakup from the indentation to the tail end is close to a thin jet of fluid due to the Plateau-Rayleigh instability.

In conclusion, he discussed validation work done on a bare plate without modeling recoil or the Marangoini effect, by comparing to experimental results (Gusarov et al., 2009). He and his collaborators found that the bare plate melt pool compared well with experimental results, although the model used an average value for the material absorptivity. The simulation and experimental results both showed the Plateau Rayleigh instability. The simulation also predicted the main characteristic of the laser powder track. The melt pool diameter and height also match experimental results, although the melt pool depth was underestimated. Once the recoil and Marangoini effect were added to the model, the melt pool depth estimate more closely represented experimental findings.

Discussion

Neil Hodge, Steve Daniewicz, and Saad Khairallah participated in a panel discussion following their presentations, moderated by Wing Kam Liu. An audience member posed the first question to Khairallah about the numerical methods used for the simulation he described (i.e., mesh strategies, time integration, spatial resolution, and governing equations). Khairallah responded that the simulation he described was done using LLNL's ALE3D code, with many of the technical details available in Khairallah and Anderson (2014). He stated that the simulation is Eulerian with thermal-hydro coupling with conventional governing equations and uses an unstructured mesh with a high resolution (approximately 3 microns) to capture the point contact and heat interactions of the particles.

A participant asked about the computing resources applied to the LLNL simulations. Hodge said their SLM Diablo code ran on the order of hundreds of hours with hundreds of central processing units. Khairallah said their ALE3D simulation runs on the order of tens of thousands of hours. He noted that the implication of these long run times is that not all researchers can conduct these types of simulations, but there are many opportunities for less computationally intensive research in these areas.

Another participant asked Daniewicz about the need for more and better elastoplastic constitutive modeling: What is the state of the art in this area and what is needed? Daniewicz commented that what is needed is to build in the unique microstructures that were not part of the fusion welding research. The participant responded that the physics community is developing similar physics-based models and there might be some opportunities to link these communities.

A participant asked Khairallah if the powder distribution in the ALE3D simulation was uniform and if a distribution of powder sizes would impact cavity generation. Khairallah responded that any distribution could be used but he and his collaborators have not examined if the powder distribution impacts cavity generation. Liu commented that experimental techniques to lay down the powder bed are an open research area and expanding the ALE3D simulation to include oxidation could provide an opportunity to examine fatigue. Khairallah responded that the physical parameters for oxidation would be needed to do this since the surface tension significantly changes. The community urgently needs access to realistic data to input into models, Khairallah stated.

A participant asked if the panelists had any comment on the hypothesis that small voids (less than 5 microns) in materials come from preexisting voids in the powder particles. Khairallah commented that simulations indicate that the voids in the particles can exist in the shallow pools. He said that many other possible hypotheses to this issue exist. Another participant asked which codes are open source and what codes would be good to start with for AM modeling. Hodge responded that, to his knowledge, none of the LLNL engineering codes are open source but there have been efforts to make the computing resources more accessible. However, partnerships between academia and LLNL are possible. Khairallah stated that each code has a different policy but LLNL is making an effort to interface better with industry by sharing codes and computational capabilities.

In response to a question about how much computing on graphics processing units (GPUs) could speed up calculations, Hodge stated that solving linear algebra is a hindrance for implicit finite element simulations. He has not seen any cases of highly parallelized linear algebra solvers on GPUs and suspects this will continue to be an issue until the linear algebra packages are updated to run on GPUs.

Daniewicz was asked by Liu how the community can work with ASTM, industry, NIST, and others to advance standards. Daniewicz stated that ASTM is focused on coupon testing so a first step could be to use high-performance computing to connect the coupon testing with the component behavior. A participant wondered how new processes can be handled within established standards. Daniewicz responded that this is an important topic because establishing standards for quickly developing fields is challenging (see Figure 2-4).

Lastly, Liu asked about how non-destructive evaluations can help with in situ modeling as well as examining residual stress and other effects. Daniewicz commented that he typically uses non-destructive evaluations to examine defects; however, there is an opportunity in AM to further the use of these tools to do real-time process control and monitoring.

3

Computational and Analytical Methods in Additive Manufacturing

The second sessions of the first two days of the workshop provided an overview of novel computational and analytical methods for fully characterizing process-structure-property relations in additive manufacturing (AM) processes for materials design, product design, part qualification, and discovery/innovation. This includes multiscale modeling, computational materials, modeling topology optimization, verification and validation methods, and uncertainty quantification for AM processes and AM resulting materials.

Anthony Rollett (Carnegie Mellon University), Wayne King (Lawrence Livermore National Laboratory), Corbett Battaile (Sandia National Laboratories), David Snyder (QuesTek Innovations), Gregory Wagner (Northwestern University), and Joe Bishop (Sandia National Laboratories) each discussed research, challenges, and future directions relating to the following questions:

- What are computational methods and approaches for simulating materials processing, properties, and performance relationships for materials design using AM as well as key process parameter identification and process mechanics?
- How can high-performance computing spanning scientific discovery be leveraged with ensembles of engineering solutions?
- How can topological design loops be integrated with AM processes and mechanics within a computational framework?

- How can AM benefit from fundamental advances in verification, validation, and uncertainty quantification methodologies?
- What analytical, experimental, and software tools are needed?
- How can new tools be integrated to impact adoption of AM?
- What opportunities exist for high-performance computing in order to provide fundamental scientific discovery of the process-properties-performance relationship relevant to AM?
- What are the drivers and the fundamental advancements needed for computational methods and optimization techniques?

COMPUTATIONAL AND ANALYTICAL NEEDS IN ADDITIVE MANUFACTURING

Anthony Rollett, Carnegie Mellon University

Anthony Rollett began by adding two additional questions to the session topics that he believes should be considered:

1. Is there sufficient funding in the United States for fundamental research and development for AM?
2. Most U.S. academic institutions house their AM programs in mechanical engineering departments, and materials departments remain largely disengaged. How can we better involve materials science and engineering students and faculty in AM?

He then showed a video of direct metal AM to illustrate the geometric complexity, the relationship between the melt pool and the previous layers, and other complicated dynamics at play in AM. Carnegie Mellon University (CMU) has a NextManufacturing Center with equipment for AM with metals and polymers, as well as metrology. CMU encourages industrial partners to use this equipment on a fee basis while also providing training on AM equipment.

The state of the art for direct metal AM is advancing, according to Rollett. While there are some estimates indicating that AM parts are not cost-effective versus traditionally manufactured parts, he noted that these often ignore the time savings that AM can provide. Most three-dimensional shapes can now be additively produced directly out of metals with nearly 100 percent density and features down to 200 microns. Parts with volumes up to 10 in × 10 in × 8 in can take from a few hours to over a day each to build. AM parts are currently being used commercially, including a GE fuel nozzle and other parts going into commercial jet engines. The current processes were developed to allow shapes to be built but there can be significant residual stress in as-built parts. Certification and qualification are non-trivial considerations since the materials can vary in their microstructure and defect structure compared to conventionally manufactured parts. CMU is mapping all direct metal processes across their alloy systems, Rollett explained, noting their results can differ due to varying thermal properties.

He commented that almost all metal manufacturers are considering direct metal AM. A crucial step to identifying components as good or bad for AM is to map part specification to AM technical capabilities. While AM benefits are most notable when parts are redesigned specifically for AM, it typically takes users 6 to 12 months to become proficient in AM techniques. He commented that understanding simple trends in processing behavior can have a notable impact. Rollett illustrated this point using a beam power versus beam travel speed map for an electron beam process to infer process behavior. In particular, build rate scales with power, process precision scales with melt pool size, and the beam can stay on straight lines while increasing power to maintain precision and increase build rate. He emphasized that a road map such as this does not give a user all the necessary information, but adding information can help fill in some of the gaps.

There are several challenges when working with AM powders, Rollett explained. First, specific AM approaches require small powder particles but the majority of powder produced is larger than the machines can use. He commented that the community needs a better understanding of fluid flow to optimize production of small powder. Cost is also a concern as Ti-6Al-4V powders for machines cost approximately $250-650/kg and commonly contain voids that can lead to porosity in parts. There is little room for competition because powders have to be purchased from the manufacturers to uphold equipment warranties. An approach to reducing costs, he stated, would be to explore the use of larger size powders in an application that allows rougher surface.

Powder characteristics are related to flow behavior, and Rollett stated it is important to realize that powder particles are often irregularly shaped with satellites attached and other abnormalities and can have unexpected size distributions. These size differences are not necessarily detrimental to AM and can actually improve the process in some situations. He noted that the modeling community could assist in improving control of powder production.

Pores (including voids in particles, keyhole defects, and incomplete fusion) are common in most materials, even those not typically associated with porosity (e.g., stainless steel), and can affect long-term fatigue performance (Magnusen et al., 1997). Prediction of porosity is a complex problem because the geometry of melt pools is complex; the pools overlap across layers, and there can be regions of unmelted material resulting in lack of fusion porosity. However, models are being developed that appear to match well with experimental data (Ming, Pistorius, and Beuth, 2015).

Rollett raised two issues of importance for AM: variability and fatigue measurements. Variability can come from a variety of sources, including local part geometry and melt pool size and shape, and can have significant ramifications for part reliability and reproducibility. He mentioned the importance of comparing fatigue resistance and strength of AM parts with those produced by traditional manufacturing (Juvinall and Marshek, 2006).

Rollett reiterated that the microstructures of AM parts can vary from those of traditionally manufactured parts. In particular, the melting and cooling process and post-build heat treatments can transform the microstructure, and it is important for users to realize that materials with these different microstructures will respond differently.

Lastly, Rollett emphasized that advanced AM experimental capabilities often require supercomputer resources for data reduction, reconstruction, and analysis. He stressed that these challenges cannot be underestimated. However, analyses of smaller data sets can pose their own challenges as well. In conclusion, Rollett offered the following suggestions in response to the overarching session questions:

- Heat, fluid, and particle flow; stress-strain including crystal plasticity; and computational thermodynamics are key computational methods and approaches for simulating AM materials processing, properties, and performance relationships.
- High-performance computing can be utilized to enhance AM-specific capabilities and validate codes against experiments.
- Computational approaches to understanding AM processes and mechanics may require a multiscale approach.
- AM can benefit from improvements in real-time data access via data analytics and state-of-the-art characterization.
- High-performance computing offers the potential for both analysis of large-scale experiments (e.g., synchrotron X-rays) and large-scale simulations with ever-increasing resolution.

- There is likely insufficient U.S. funding for fundamental research and development for AM.
- Research funding as well as internships and scholarships directed at AM could help engage materials science and engineering students and faculty in AM.

He highlighted the following objectives as being important to the AM community:

- Integrating, scaling up, and homogenizing detailed modeling of heat, fluid, and energy flows into reduced-order models;
- Setting up data sharing that is useful for data analytics but also fair to the groups that contribute the data;
- Supporting industry with basic research that impacts practical issues (e.g., powder manufacture, qualification);
- Incorporating materials microstructure (e.g., orientation, lattice strain) into continuum codes; and
- Utilizing big data techniques to deepen the validation process (e.g., use reconstructed images or diffraction data).

HIGH-PERFORMANCE COMPUTING AND ADDITIVE MANUFACTURING: OVERCOMING THE BARRIERS TO MATERIAL QUALIFICATION

Wayne King, Lawrence Livermore National Laboratory

Wayne King began by referencing a recent survey in which 42 percent of companies indicated that poor part quality is a barrier to adopting AM. He stated that modeling and simulation are foundational to qualification, but it is not always obvious how to approach this important part of the process. The work King presented was a collaborative effort[1] at LLNL over the last few years.

Modeling of the AM process began in 1998 and included metal thermal modeling (Contuzzi, Campanelli, and Ludovico, 2011; Dai, Li, and Shaw, 2004; Kolossov et al., 2004; Roberts et al., 2009), metal thermo mechanical models (Hussein et al., 2013; Matsumoto et al., 2002), polymer powder-bed fusion (Williams and Deckard, 1998), residual stress modeling (Zaeh

[1] Collaborators include Wayne King, Andy Anderson, Robert Ferencz, Neil Hodge, Chandrika Kamath, Saad Khairallah, Ibo Matthews, and Sasha Rubenchik.

and Branner, 2010), and laser-powder interaction (Fischer et al., 2003; Gusarov and Smurov, 2010; Tolochko et al., 2003). King commented that much of this work has been concentrated outside the United States.

Modeling metal AM processes is challenging because a broad range of length and time scales are covered. King explained that LLNL researchers use multiscale modeling approaches to provide key insights into AM metal processes that will inform performance simulations. The goal is to link powder, microstructure, and process-aware models through information-passing to inform a performance model and an effective medium model, as shown in Figure 3-1. The powder model and the effective medium model (on the scale of the part) were the focus of this presentation.

The effective medium model that King and his collaborators developed utilizes LLNL's high-performance computing Diablo code (Hodge, Ferencz, and Solberg, 2014). Diablo facilitates prediction of material behaviors on the scale of the part and is suitable for complex structural response and temperature-driven deformations. He showed an example of a simulation of building a cubic centimeter cantilever part to design a residual stress sample. He commented that there are a number of alternative approaches to doing part-level thermo mechanical models, including custom codes (Denlinger and Michaleris, 2015; Pal et al., 2014; Neugebauer et al., 2014a; Neugebauer et al., 2014b) and commercial codes (Schilp et al., 2014; Seidel et al., 2014; Krol, Branner, and Zaeh, 2009).

The powder-scale model developed by King and his collaborators uses the ALE3D code to perform a first full-physics simulation of laser powder-bed fusion. The physics incorporated include melting and solidification, solidification shrinking, phase transformations and separation, multistructural evolution, convection, heat conduction, radiation, absorption, vaporization, capillary forces, Marangoni convection, gravity, powder layer, and wetting and dewetting. He explained that first principles calculations are being used to understand the absorptivity of the metal powder. The powder size (typically tens of microns) is much larger than the laser wavelength (1 μm), so ray tracing can be used. The refractive index of the metals involved is known or can be measured. On each reflection, the absorption is determined by Fresnel formulas, which include angular and polarization effects. Multiple scattering plays an important role.

Using the commercial code FRED[2] for ray tracing with considerable

[2] The website for FRED software is http://photonengr.com/software/, accessed August 16, 2016.

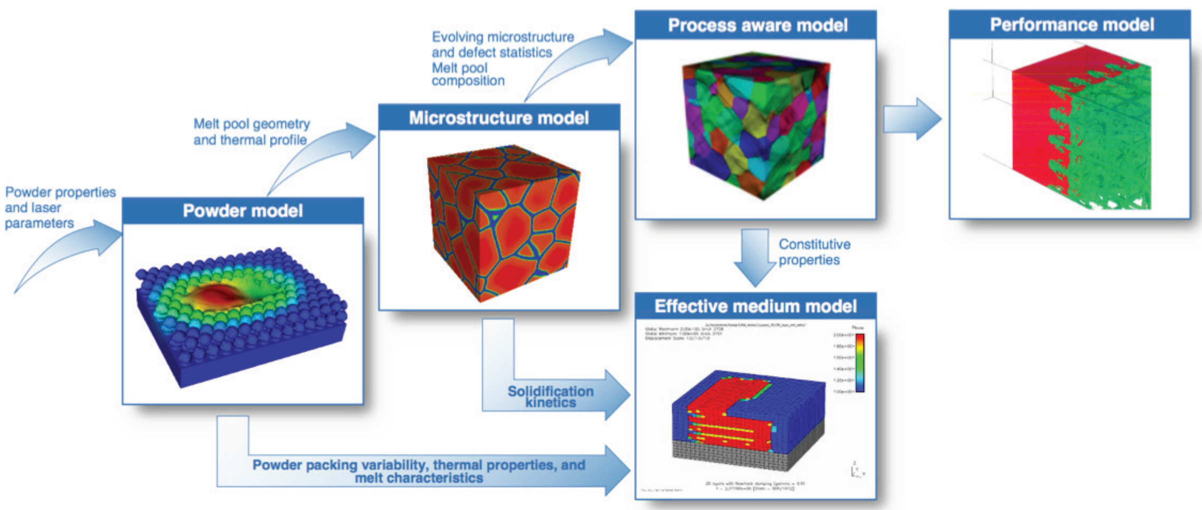

FIGURE 3-1 Multiscale modeling approaches for metal additive manufacturing. SOURCE: Wayne King, Lawrence Livermore National Laboratory, presentation to the workshop.

post-processing, King explained that approximately half of the energy is absorbed by the top layer of powder particles, nearly half of the energy is reflected, and only a small portion of the energy leaks through to the underlying layer. Recoil pressure, he explained, occurs when the laser hits a powder particle and the particle quickly reaches the boiling point. The particle rapidly starts evaporating and the evaporating metal jet exerts a force on the liquid, pushing it out of the laser path, therefore allowing the laser to reach the substrate. Using mesoscopic three-dimensional simulations that integrate recoil pressure, King and his collaborators showed that thermal conductivity is a small contributor to the melting process compared with the effects of the recoil pressure.

There are alternative approaches to simulating this as well, King noted, including two-dimensional Lattice Boltzmann methods (Klassen, Scharowsky, and Körner, 2014; Körner, Attar, and Heinl, 2011; Körner, Bauereiß, and Attar, 2013), three-dimensional open-source models (Gurtler et al., 2013), and three-dimensional discrete element methods (Ganeriwala and Zohdi, 2014).

Simulation uncertainty quantification and experimental comparisons are an essential component to AM modeling, King stressed. Experiments can reveal missing physics in simulations. He showed an experimental video similar to the setup of the ALE3D powder simulation. Experiments show the melt pool expansion exerts a forward push on powder and the nearby powder is consumed through capillary forces into the melt pool, similar to the simulation. However, non-local powder experiences inward force toward the melt pool, unconsumed cold powder is swept backward and upward, and molten droplets eject in both directions directly from the melt pool. Experiments also observed a forward ejection at high scan speed and high power and a faint vapor trail at higher power.

He also discussed options for improving efficient predictions, including combining advanced sampling with a Gaussian process code surrogate. This has the potential to more quickly highlight regions of power and speed space that could be viable, therefore making further studies more effective. In conclusion, King summarized the issues and challenges in powder and part-scale models. The powder model needs the following:

- A better laser absorption model,
- An approximation of some physics,
- Thermophysical properties over a broad range of temperatures,
- Fine zoning,

- Explicit time marching to limit time step,
- Experimental data, and
- Inclusion of evaporation and flowing cover gas effects.

The part-scale model has the following challenges:

- Disparate spatial scales of the laser energy source and the overall part geometry,
- Disparate time scales of local heating versus overall heat transfer and the actual time of fabrication, and
- Scant handbook-type property data available for high temperatures.

REVOLUTIONS IN DESIGN AND MANUFACTURING: TOPOLOGY OPTIMIZATION AND UNCERTIANTY QUANTIFICATION IN ADDITIVE MANUFACTURING

Corbett Battaile, Sandia National Laboratories

Corbett Battaile began by noting that his presentation would focus on design, specifically his team's work at Sandia National Laboratories.[3] He explained that topology optimization is a way to determine an optimal shape to best achieve a set of desired objectives, performances, or specifications using a distribution of materials and set spatial constraints. Traditional manufacturing sets constraints on how manufacturing is approached, but these constraints are loosened for AM. The design process can therefore take a more prominent role with AM than it has had in traditional manufacturing. He showed an example of a lantern bracket designed via topology optimization, where the material and the spatial constraints were defined and the shape was developed to optimize mechanical characteristics and behavior.

Design for traditional manufacturing has been revolutionized in recent decades, moving from drafting by hand to computer-aided design (CAD). Now, advances in manufacturing are furthering design capabilities, including the establishment of the Plausible Topology Optimization program (PLATO), developed at Sandia National Laboratories. The goal for design of AM parts mirrors AM motivations in general, Battaile explained, including the desire to be affordable, agile, and assured. This new design flexibility

[3] Collaborators include Miguel Aguilo, Ted Blacker, Andre Claudet, Brett Clark, Ryan Rickerson, Josh Robbins, Louis Vaught, and Tom Voth.

affords many great opportunities, but significant challenges include in situ material qualification and characterization, specifically how to address and integrate the process-structure-properties hierarchy for this new class of materials with complicated microstructures.

The utilization of topology optimization is an inversion of the conventional design paradigm, which in turn leads to an inversion of the qualification process. As an optimizer is designing a part, Battaile explained, it is doing the continuum analysis to qualify the design as it is evolving. In conventional manufacturing, a form is specified, designed, and then verified using finite element analysis, iterating as needed. Using topology optimization, the design domain and function are first specified, topology optimization using finite element analysis determines the form that meets the function, and then an optimized design is established. Performance prioritization can then be done to define a Pareto suite of topologies evaluating the thermal mechanical properties of the proposed topologies.

Advantages of topology optimization for manufacturing include the opportunity for increased complexity, minimal waste, fast design to manufacturing time, and mixed and graded materials. AM is moving toward point-wise material variability and the optimization needs to be able to account for this when developing the design. Battaile commented that in situ metrology to validate designs could also be built into the optimization process, keeping in mind the computational cost constraints.

To illustrate the point about computation time, Battaile discussed an idealized linear static problem with 1.5 million elements, one objective (to maximize stiffness), one loading condition, and built-in uncertainty quantification. This problem would take approximately 2,000 hours (or 12 weeks) to solve with approximately 4,000 processors, he explained. Researchers at Sandia are looking into ways to reduce this run time using physics-based reduced-order modeling to reduce the finite element resolution and smart sampling techniques to streamline the uncertainty quantification, which can reduce the runtime to approximately 5 hours.

Many steps need to come together to make this approach usable for engineers, he emphasized. The function-based design environment is dependent on a variety of inputs and analyses, as shown in Figure 3-2. A number of tools can be used at each of these steps. Battaile summarized that in topology optimization tools, high fidelity in a modern design and analysis environment with smooth connected shapes and fast convergence is key. Interactivity is important, especially with speed and control, to develop robust designs that can be directly printed and interfaced to a CAD system.

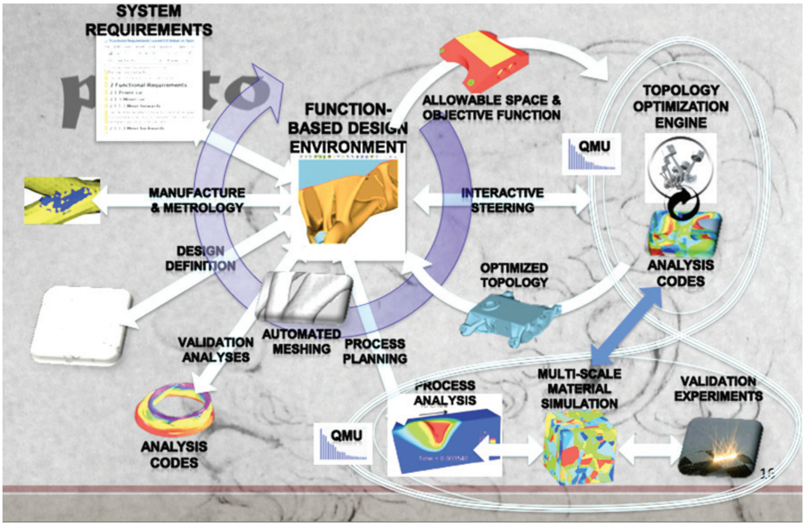

FIGURE 3-2 Function-based design environment. SOURCE: Corbett Battaile, Sandia National Laboratories, presentation to the workshop.

Discussion

Following their presentations, Anthony Rollett, Wayne King, and Corbett Battaile participated in a panel discussion moderated by Steve Daniewicz from Mississippi State University. A participant noted that transferring topology optimization design back into CAD tools is often challenging. Battaile agreed that this is essential; he said they use a tool that is part of Sandia's CUBIT software,[4] and they are working on exporting the geometry directly to CAD software.

Another participant asked if the laser sintering modeling King described includes the possible effects of ionization, which would then create an electrical plasma that could have the forces to produce the motion of the particles. King clarified that the current simulation does not include this force and his impression is that to do so would require a finer resolution mesh and time steps. However, he stated that they know that a plasma pool does form and it would be beneficial to simulate this effect. Rollett added that King's simulation involved a laser powder bed and, in contrast,

[4] The website for the CUBIT toolkit is https://cubit.sandia.gov/public/tutorials.html, accessed August 16, 2016.

the electron beam powder bed is typically preheated to sinter the particles together, which would likely lead to very different results.

A participant referenced the intensive computation power required for simulations and noted that even the reduced computational time discussed would still be prohibitive for many researchers. He asked what resources are necessary to make these simulations available to the wider community. Battaile emphasized that this is a major challenge but, fortunately, tools for speeding topology optimization are being developed and computing resources for researchers are growing. He said that much of the promise is not just in taking a finite element analysis and doing a topology optimization on it but rather in integrating this capability with process modeling and material physics calculations. An audience member mentioned that reduced-order modeling holds great potential but has not been widely applied to AM yet. King commented that the goal is to build parts computationally in less time than it takes to build parts physically. Rollett noted that advances in this area will likely depend on a multiresolution approach.

A participant asked how the cm^3 model King described is connected with the powder-scale model and why the laser in the cm^3 model is wider than he would expect. King responded that the models are linked by information-passing between them. The laser appears large because that is the mechanism by which the models homogenized information-passing. They simulated thick layers with a large laser beam in order to simulate the cm-scale part in a reasonable amount of time.

An online participant asked how access is granted to operators of commercially available machines to obtain and control process parameters (e.g., laser path, beam power and travel speeds). Assuming an AM process can be optimized virtually using numerical simulation, the participant asked if optimized process parameters such as the new laser path or laser power could be readily deployed into the machines. Rollett commented that it would be useful if these parameter values were easier to obtain. Manufacturers protect some information for proprietary reasons, but some open-source machines are being developed. He believes there is hope for optimizing the AM process by treating it as a black box response function since the inputs and outputs are known.

Another participant posed a question to the panel about whether the ray tracing approach is materials-specific and can thus be incorporated in a mathematical model. King stated that while only the complex index of refraction of the material is needed to do the ray tracing approach, this is unknown for many materials. Also, ray tracing works well for some systems (e.g., titanium and stainless steel) but not others (e.g., aluminum). As the laser beam moves, the powder is quickly converted to liquid so the absorptivity of the liquid is the key parameter, not the absorptivity of the powder. For the part-scale model, a volumetric heat source is being considered. A participant asked if the ray tracing approach can be translated to particle size modeling using ALE3D. King said this is already being implemented into the model through a ray-tracing package.

A participant asked how important uncertainty quantification is and if it is related to the final quality of the product or part and in situ monitoring (e.g., data mining, reduced-order modeling). Rollett noted that parts are already being produced successfully with AM and reduced-order modeling is working well, and he questioned whether more detailed modeling is needed. He explained that there is a clear trade-off between tweaking process parameters and the ultimate quality of the part, but there are not clear limits about what could be done. Improving parts can be approached from the top, by bounding variability, or from the bottom, by providing the tools that make the analysis more quantitative. He also mentioned that data mining and data analytics techniques are crucial for understanding the microstructure and other parameters and should continue to be examined.

A participant commented that the computational time of topology optimization is continuing to decrease with advanced computational techniques and resources and that near real-time optimization is possible in the immediate future. Battaile agreed that this is true in a general sense but the metrics can still be intimidating. He clarified that the simulations he discussed are conducting on-the-fly conformal surface meshing in an integrated multiphysics code, which can be computationally costly. There are much more cost-efficient computational approaches to conducting topology optimization, but they may not incorporate the same features and physics.

A participant from a national laboratory asked if the optimization algorithm accounts for either nonlinear geometric constraints (e.g., contact) or processing constraints (e.g., process-dependent residual stresses). Battaile said that he does not believe nonlinear geometric or processing constraints are accounted for at this time. Part of the complicating factor for the geometric constraints is that the topology optimizer starts with a dispersion of material density and then begins to move this around to decide on a shape, so nonlinear constraints are difficult to handle in the mechanical calculations.

The same participant asked if the initial mesh specification could limit the ability of the algorithm to modify the mesh. Battaile said that he is not aware of initial mesh limitations. He and others are currently working to develop adaptive meshing and there have not been any indications of issues. An audience member commented that new generalized finite element and measurement methods may be helpful. Rollett noted there are also image-based techniques that remove the need for a mesh.

Another online participant asked Battaile if the decoupled inverse problems of design, manufacturing, and uncertainty quantification can be combined. For example, could the cost and time consumption of AM and the AM design limitations all be considered in the design process? Or, could the design and manufacturing process be updated on the fly as uncertainties are detected by real-time metrology? Battaile responded that combining design, manufacturing, and uncertainty quantification is an open challenge. Rollett commented that there are a number of related issues from the control perspective that need to be addressed as well. Battaile noted that on-the-fly metrology that connects back with the design process would be a powerful capability.

A question was asked about the connection between simulations and in situ monitoring and measurement. Specifically, the participant noted that experimentalists often view simulations as a way to better understand what was observed experimentally, but the emerging predictive capabilities of models suggest that the community may benefit from adjusting in situ measurement strategies to try to observe phenomena that models are predicting. He wondered if this is a trend in the AM community. King stated that measuring predicted behavior is important but he believes the modeling and simulation could make the most impact in feedback control to enhance the overall quality of AM parts.

A participant commented that hydrodynamics might be important and wondered if King has examined the chemistry of the gas moving backward in his simulation. King agreed hydrodynamics are important and stated there is interplay between the cover gas and the plasma that is being formed. He and his collaborators are hoping to conduct plasma diagnostics to help understand this behavior. The participant asked if the particle size impacts the particles moving toward the melt pool, but King has not examined this area yet. Lastly, the participant asked if the shape of the laser beam impacts defect formation. King stated that a Gaussian laser beam is a poor choice because the boiling temperature will be reached at the center of the beam, and they are examining several other beam profiles.

There was a comment that AM allows for a highly non-uniform material distribution, which works for optimization but is a challenge for structural analysis. Battaile agreed that one of the key issues is understanding when the scale thresholds are crossed and how to deal with scale-specific considerations. He said an open challenge is tying the analysis and physics models across scales to do on-the-fly design.

APPLICATION OF INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING TO THE DESIGN AND DEVELOPMENT OF NEW HIGH-PERFORMANCE MATERIALS FOR ADDITIVE MANUFACTURING

David Snyder, QuesTek Innovations

David Snyder mentioned that computational methods and approaches for materials design and integration would be the focus of his presentation, specifically with respect to computational thermodynamics and mechanistic property modeling. He emphasized the role of materials and process design as well as integrated computational material engineering (ICME)-based qualification for integrating analytical and computational tools.

He began by explaining that QuesTek focuses on applying a computational thermodynamics approach toward alloy and process design, mostly to simulate phase transformations (e.g., solidification and solid-state precipitation and recrystallization) and microstructural constituents (e.g., strengthening phases, impurities, evolution during complex thermal cycling, and post-processing). This type of approach covered multiple length scales, from atomistic density functional theory calculations to macroscale solidification behavior. He explained that the design parameters (e.g., the matrix, strengthening dispersion, grain refining dispersion, austenite dispersion, and grain boundary chemistry) can help link the process variables with the functional requirements.

AM materials respond differently to processing than their conventionally processed counterparts, Snyder noted. There are unique microstructures in both as-built and post-processed conditions, and post-processing responses are driven largely by the complexity of thermal history and the magnitude of residual stresses generated by process. He stated that existing alloys and post-process conditions are not optimized for AM-specific behaviors, resulting in complex microstructures and unreliable AM performance. Snyder highlighted select metallurgical phenomena that need to be considered for different areas of the AM process flow. For raw stock production, he mentioned the impact of exogenous powder contaminants (e.g., oxides) in the stock as a unique AM challenge. For AM processing (e.g., SLM, EB), solidification defects such as hot tearing and incipient melting are a concern, as is quench suppressibility (e.g., cold cracking and transformation stresses). For the post-heat treatment response (e.g., stress relief, HIP), he stressed that additional optimization is needed for recrystallization response (e.g., grain and phase refinement) and precipitation response.

To illustrate these concepts, Snyder provided a couple of case studies from QuesTek. The first was a nickel superalloy study illustrating that residual stresses can drive recrystallization during post-processing. He commented that established materials and processes are not optimized for AM-specific recrystallization response. While there are opportunities to design alloys and processing to tailor behavior for AM, more information is needed to better link models.

The second case study used a titanium alloy (Ti-6Al-4V) to illustrate that proper design of microstructures is critical to predictability and reliability. Current titanium relies on equiaxed, uniform microstructures for strength and ductility. Alloys have been optimized for wrought processing but unique AM microstructures emerge from cooling-rate sensitivity, resulting in substantial variations in a single build. Better understanding the material response is essential but is difficult to model. He emphasized that there are opportunities to use titanium alloys in a way that is more predictable, reliable, and isotropic than what has been observed with Ti-6Al-4V.

The third and final case study he discussed highlighted AM of high-strength aluminum, which is currently limited by hot tearing phenomena where cracks form during the build process. This phenomenon is driven by high residual stress and suboptimal solidification behavior. Currently, aluminum is restricted to low-performance alloys designed for casting since the high-performance alloys designed for forging are not amenable to AM. He stated that there are opportunities to integrate residual stress prediction with solidification theory and design new AM-specific alloys that address crack susceptibility. He elaborated on a project at QuesTek to tailor a new aluminum alloy (Al-Zn-type) to AM needs. Computational optimization between hot tearing susceptibility (processability) and precipitation strengthening (performance) is being used to tailor material behavior.

Snyder highlighted the importance of understanding rare defects associated with exogenous powder contaminants. These inclusions and contaminants are expected to be a confounding factor for fatigue. Many oxides cannot be broken up by the lasers (Thijs et al., 2013; Louvis, Fox, and Sutcliffe, 2011) so process modeling and optimization techniques are needed to mitigate the effects of exogenous defects beyond the impact of porosity, which is being studied.

Snyder also mentioned some computational needs. One issue is that some alloys (e.g., Ti-6Al-4V) are highly sensitive to the AM process; therefore, linkage between process and microstructure is critical. Another issue discussed was select process-microstructure modeling needs, including the linkage between AM process models and solidification theory (e.g., columnar-to-equiaxed transition, cellular-to-dendritic transition, and transformation kinetics), location-specific thermal history (e.g., input into solidification models and phase evolution models), and residual stresses (e.g., input into recrystallization models). He emphasized that better physical understanding of AM processes can drive targeted materials design for more predictable AM components.

Once there are predictable and reliable materials, computational approaches exist to accelerate qualification. The current ICME approach to accelerated qualification of new material and processes couples well-calibrated, mechanistic property models with predictable sources of processing variation to project location-specific properties and design allowables. He suspects these types of coupled approaches will be critical for AM because the AM process is expensive and would benefit from computational experimentation. However, near- and long-term issues exist with applying these approaches to AM. In the near term, process variables that are primary sources of variation are well known in conventional processing but not for AM. Researchers need validated AM process models to provide input into true sources of AM-specific process variation before such methods can see full utilization, he stressed. The AM process is also highly material dependent and is driven by the response to post-processing. A long-term issue is that qualification for AM is really qualification for parts.

Computational advances in AM are crucial for widespread industry adoption, Snyder argued. The physical understanding of how material behaves during AM processing is key to establishing confidence for implementation in industry. Current adoption is restricted by this lack of understanding, and fundamental modeling can shed light on the physics of process to increase industry confidence. He said that modeling can help to down-select key variables for more targeted experimentation. He also argued that coupling in-process monitoring and modeling within an ICME framework is critical for robust production, especially given the significant sources of variability in AM processes. Models that define select quality metrics and are implemented with in-process monitoring to establish confidence intervals would be helpful.

In conclusion, Snyder summarized that predictable materials are needed to enhance build reliability, reduce sensitivity to AM process variables, allow tailored microstructures (e.g., mitigation of AM anisotropy, design for AM-specific defects such as inclusions, and exploitation of AM-specific responses such as rapid solidification and recrystallization), and simplify computational approaches. He suggested that materials design theories are available, but a comprehensive understanding of what makes any material "well-behaved" for AM and how process model insights can facilitate AM materials design is needed.

COMPUTATIONAL AND ANALYTICAL METHODS IN ADDITIVE MANUFACTURING: LINKING PROCESS TO MICROSTRUCTURE

Gregory Wagner, Northwestern University

Gregory Wagner began by discussing linking modeling and simulation of process to performance. He explained that the impacts of process parameters (e.g., laser power, scan speed, scan direction, material, powder size, and layer thickness) and the microstructure (e.g., porosity, grain structure, surface roughness, precipitates, voids, defects, and residual stress) on properties and performance (e.g., strength, fatigue life, ductility, hardness, and toughness) would be the focus of his presentation.

He noted that computational methods and optimization techniques are difficult for AM because of multiple length and time scales, complicated or unknown physics models, and complex moving interfaces. In a typical AM approach for metals (e.g., laser engineering net shapes [LENS], selective laser melting [SLM], or electron beam melting [EBM]), multiple analyses are important, including the following:

- Powder delivery, using either a feed or bed formation;
- Heat source, utilizing either a laser or electron beam;
- Part scale, incorporating heat transfer, phase change, and thermomechanics;
- Powder and sub-powder scale, including melting and solidification, deformation and flow, and microstructure formation; and
- Mesoscale, focusing on homogenization to connect the part scale and the powder and sub-powder scale.

AM phenomena occur on multiple time and length scales, Wagner commented, which impose serious trade-offs between solution resolution and computational efficiency of simulations. He discussed a method for concurrent multiscale modeling that focuses on the macroscale and simulates the microscale only where needed (e.g., where stress is concentrated or a feature such as an overhang is present). The concurrent approach allows the complicated thermal history and other factors to be imposed on the microscale while also bringing microscale information into the macroscale. This approach can take the form of coupling the part-scale model with what is happening at the melt pool or particle scale.

He gave an example of coupling the macroscale finite element simulations with microscale Thermo-Calc simulations. Thermo-Calc can give properties (such as the enthalpy versus temperature curve) based on composition by solving the local phase evolution or diffusion problem. He showed two simulations comparing a finite element simulation with properties derived through Thermo-Calc, demonstrating the part-scale sensitivity to the microscale.

The goal is to extend this type of coupling to handle the microscale problem by using a multidimensional phase field model to get the solidification structure, he explained. Since large thermal gradients lead to complex microstructure evolution during manufacturing, the local thermal history is used to predict the microstructure. This concurrent multiscale method is approached with fairly simple isotropic phase field models that track the solidification front but will hopefully allow anisotropic microstructure and dendrite formation to be simulated. He emphasized that modeling these phenomena will give greater insight into process control.

Full fine-scale modeling of a part is unrealistic but, according to Wagner, there are opportunities to utilize high-performance computing with reduced-order modeling techniques. This may involve pre-computing large-scale simulation to compute mode shapes for fast approximate solves (Carlberg et al., 2013) or nonlinear dimensionality reduction (or similar methods) to classify and query databases of fine-scale solutions (Tenenbaum, de Silva, and Langford, 2000). To illustrate the complicated and unknown physics models, Wagner gave the example of modeling e-beam heating. He explained that the correct form of the thermal source term due to beam heating is unknown but Monte Carlo simulations of electron-atom interaction may elucidate this (Yan et al., 2015).

In terms of tools for AM, he commented that non-isothermal, multi-component phase field models for solidification of complex materials are needed. These could be used to examine phase field simulation of martensitic transformation under plastic strain (similar to work done by Kundin, Pogorelov, and Emmerich, 2015). Additional mesoscale models for powder beds with different levels of particle consolidation would also be helpful (e.g., Zhou et al., 2015).

Dealing with model uncertainty is another consideration. Several key parameters in AM are still not well understood, Wagner commented, including how high the temperature gets during AM. He stated the modeling community could do more to help determine what quantities that can be measured will best inform model selection. However, verification of macroscale thermal models is challenging as meshes are refined to the particle scale. Verification needs to be better defined in these cases, he stressed.

Complex moving interfaces are another consideration. He noted that important physics include melting, solidification, flow, vaporization, pore formation, surface tension, conduction, convection, radiation, thermo-capillary motion, and dendrite formation. It would be helpful to be able to combine detailed simulations to capture the evolving interface in a way that is easier to model and run. He commented that progress is being made on modeling powder melt and solidification (King et al., 2015; Markl et al., 2015). Wagner and his collaborators are developing a conservative level set approach to simulate the motion of the liquid vapor interface while simultaneously using a phase field method to track the solid-liquid interface. Conservative level set methods are being used for simulations in multiphase fluid dynamics (Desjardins et al., 2008) and phase field models for fluid-gas interaction (e.g., Kim, 2012; the work of A. Yamanaka at Tokyo University of Agriculture and Technology) have been used to model complex interfaces. Finite cell methods (Schillinger and Ruess, 2015) and extended finite element methods have been used for nonconforming mesh simulations of randomized microstructures (e.g., the work of Jifeng Zhao at Northwestern University). In conclusion, he summarized three main points from his presentation:

1. Interdependence between scales in AM calls for new computational methods. He noted that concurrent macroscale and microscale simulations should be possible at localized regions of interest and reduced-order models informed by high-performance computing simulations may bring real-time microscale simulations in reach.
2. Complex physics can be understood through both simulation and experiment. He noted that a coordinated validation plan between modeling and experiments is needed.

3. Methods for modeling complex moving interfaces can impact AM simulations.

ADDITIVE MANUFACTURING CHALLENGES FOR COMPUTATIONAL SOLID MECHANICS

Joe Bishop, Sandia National Laboratories

Joe Bishop stated his presentation would focus on current challenges of computational modeling for solid mechanics, as well as how AM is an interesting application for solid mechanics. He noted that he would be drawing from several projects with many collaborators, including a project on mechanical response of AM stainless steel 304L across a wide range of strain rates,[5] and the Predictive Performance Margins Project[6] designed to provide a science-based foundation for design and analysis capabilities that links nanoscale mechanisms and microscopic variability to stochastic performance. He noted that many of the simulations used the solid-mechanics finite elements analysis module within the Department of Energy's Advanced Simulation and Computing code Sierra/SM.[7]

At the macroscale, Bishop explained, researchers typically perform a component or part analysis and qualification to determine the stress field on the part. AM can follow the same approach, first by determining the complex temperature history at each material point. Then, the as-manufactured state can be calculated using an advanced viscoplastic material model with internal state variables capable of representing processing history (e.g., recrystallization), which may include results relating to the residual-stress field, initial yield stress (field), hardening, and failure. The part performance can then be predicted with error estimation and uncertainty quantification in quantities of interest (Brown and Baumann, 2012).

Bishop highlighted four key challenges and opportunities for computational solid mechanics. The first challenge is whether the concept of a material property is appropriate for AM parts. He emphasized that material property and macrostructure are no longer separable and that the process,

[5] Collaborators include David P. Adams (SNL), John Carpenter (LANL), Ben Reedlunn (SNL), Bo Song (SNL), Todd Palmer (PSU), Jack Wise (SNL), Don Brown (LANL), Bjorn Clausen (LANL), Jay Carroll (SNL), and Mike Maguire (SNL/CA).

[6] Collaborators include John Emery, Corbett Battaile, John Madison, Brad Boyce, David Littlewood, Jay Foulk, and Rich Field.

[7] The Sierra/SM Theory Manual can be accessed at http://prod.sandia.gov/techlib/access-control.cgi/2013/134615.pdf.

material, and part must all be qualified concurrently. Assessing the accuracy of homogenization theory for AM materials involves considering scale separation, texture and anisotropy, and surface effects. He said that concepts from a posteriori error estimation need to be applied to quantify errors inherent in homogenization and material-model form error.

Macroscopic homogenization, Bishop explained, is when a complex material with a unique microstructure and fine-scale fluctuations is modeled with mean material behavior. Estimating homogenized material properties is quite involved (Huet, 1990). The first step is to establish a representative volume element (RVE), typically with just a few grains in the smallest case. Displacement, periodic, and traction boundary conditions are then applied to the RVE to compute the apparent property. This step is then repeated with incrementally increased RVEs and eventually the apparent property values with the different boundary conditions converge to a deterministic effective value. Bishop explained that the complex microstructure associated with AM often means that larger RVEs are needed with uncertainty quantification estimates.

He gave an example of direct numerical simulation of multiscale modeling of an I-beam, where an equiaxed grain structure is modeled directly within the engineering-scale finite element model. This model uses crystal-plasticity material models for each grain and can incorporate as-manufactured states (e.g., texture, residual stress), but it requires a massively parallel finite element framework. He showed the von Mises stress field for both the homogenization solution and the multiscale modeling with direct numerical simulation. The results are qualitatively similar but with less detail in the homogenization solution. He then compared these results with an idealized LENS microstructure, showing additional variation. Bishop highlighted that Kinetic Monte Carlo[8] simulations can be used to generate the AM microstructures (as shown by T. Rodgers, J. Madison, and V. Tikare at SNL), which can be used to model the melt pool velocity and the shape of the hot zone trailing the melt pool's path.

The second issue he raised is that the residual-stress field must be quantified with its uncertainty. While he did not discuss this in much detail, he commented that there are many instances of this uncertainty quantification not being done. The residual stress field is often incorrectly assumed to be negligible and this can impact part behavior, especially for AM.

[8] The website for the SPPARKS Kinetic Monte Carlo simulator is http://spparks.sandia.gov//, accessed August 16, 2016.

The third issue is the use of data science in predictive modeling. He wondered if high-throughput material testing could be utilized for uncertainty quantification, statistical learning, and pattern recognition for material-failure precursors. Also, he suggested that statistical learning, pattern recognition, and emergent behavior could be applied more frequently and more vigorously to AM.

The fourth issue Bishop discussed related to fast simulations for industrial use. Discovery-type simulations are imperative but applying techniques to speed the computation (e.g., reduced-order models) makes the simulations usable for real applications. He emphasized that extremely efficient specialized computational methods are needed. There is an opportunity to break out of current CAD-analysis paradigms to focus on implicit representations of geometry and on implicit representations of approximation spaces so that the meshing process is eliminated (e.g., fictitious-domain methods, finite-cell methods, fast Fourier transform methods [Bishop, 2004], and mesh-free methods). He emphasized again that a posteriori error estimation in engineering quantities-of-interest is needed but heuristics in finite element analysis are still state of the art. In conclusion, Bishop highlighted short- and long-term goals to advance predictive methods in AM. He described the following list of short-term goals:

- Continue development of advanced viscoplastic macroscopic material models with internal-state variables capable of representing changes to microstructure due to complex processing history;
- Incorporate process modeling for full-field residual-stress state determination; and
- Create measurement and inversion techniques for full-field residual-stress state determination.

Bishop also described the following long-term goals:

- Error estimation in engineering quantities of interest for quantifying material model form error, discretization error, and homogenization error;
- Process models for microstructure predictions (e.g., KMC, phase field);
- Multiscale material models that represent microstructure explicitly (e.g., through concurrent homogenization with crystal-plasticity models);

- Development of crystal-plasticity models and advanced calibration methods;
- Data science enabled by high-throughput testing and digital-volume correlation;
- Development of implicit geometry representations and computational techniques; and
- Fast simulations tools for industrial use.

Discussion

Following the three presentations by David Snyder, Gregory Wagner, and Joe Bishop, a panel discussion was held and moderated by Steve Daniewicz. A participant posed a question on how well inclusions can be modeled and if there is the possibility to simulate multiple material powders in the matrix. Snyder commented that thermodynamic predictions are used to define the oxide content and linking this with process modeling could help address geometric questions, but this has not yet been explored. The participant asked if materials can be added for AM, and Snyder commented that his team has focused on the efficacy of precipitation strengthening for aluminum alloys. He said there are many opportunities to advance this strengthening in AM because the rapid cooling and solidification result in unique microstructures that may lend themselves well to strengthening modifications. However, some of the rare oxides that have been observed are large and it is unlikely that they can be worked around solely by strengthening the material. He suspects that there will have to be advances in material processing to help eliminate these defects.

The panel was then asked if AM could be used to grow a single crystal. Snyder commented that there has been a lot of work in dendrite growth theory from the directional solidification and single-crystal growth. Utilizing some of this theory may help, but there are cooling rate and gradient conditions with AM that pose additional challenges.

A participant raised the issue of separating the material models from scales and asked the panel to elaborate on what options were available. Bishop noted that there are anisotropic plasticity models at the macroscale but calibration and material testing is challenging. Scale separation is assumed when using the macroscale plasticity models. He said the method could be applied to a small part without clear separation of scale but the error would have to be quantified.

An audience member noted that data science approaches are often used in mechanics for linear analysis but asked how applicable these approaches are to nonlinear analysis. Wagner commented that data science has been applied in computer vision, speech recognition, and many other fields, and he believes it could be applied more broadly to nonlinear mechanics. Bishop agreed, noting that data science approaches could help identify correlations that may be precursors to failure, for example. He suggested it is a way to get more out of simulations than is possible using only traditional analysis. Liu commented that data analysis might be a way to accelerate analyses to make simulations more feasible in industry. A participant commented that signal analysis and image analysis approaches could help with pattern matching, and tools are available in other communities that can be applied to mechanics. An audience member emphasized that database management, data compression, pattern recognition, and statistical analyses are all areas that should be examined more.

4

Monitoring and Advanced Diagnostics to Enable Additive Manufacturing Fundamental Understanding

The third sessions of the workshop discussed in situ monitoring and advanced diagnostics to enable additive manufacturing (AM) fundamental understanding (e.g., metrology). AM provides a fundamentally different way from conventional manufacturing to build components. In contrast to conventional manufacturing, where metrology is executed after all material is removed, AM metrology can occur during the process and corrective actions can be taken in situ. It is expected that in-process metrology will provide a probabilistic result (quantifying quality and conformance uncertainty) instead of a binary result. Thus, metrology for AM will be interpreted and represented differently from classical metrology. Furthermore, AM processes offer the opportunity to quantify errors and correct them in-process by incorporating non-dimensional sensors, resulting in significantly different closed-loop process control systems. AM enables the manufacture of multi-material and functionally-graded material components. Such a capability will require a new set of in-process sensor tools to validate material quality, composition, and key performance parameters.

Ade Makinde (GE Global Research Center), Joseph Beaman (University of Texas), Jian Cao (Northwestern University), David M. Keicher (Sandia National Laboratories), Edwin Schwalbach (Air Force Research Laboratory), and Yu-Ping Yang (EWI) discussed the following questions:

- What are the in situ and diagnostics challenges specific to AM and what methods need to be developed?

- What new types of diagnostics and sensors are required to probe AM-fabricated materials?
- What recent advances in experimental methods can be leveraged?
- How is uncertainty analysis integrated into process monitoring and diagnostics capabilities?
- Given that AM enables the realization of both design geometry and multi-material characteristics, how should digitally-compatible computational and design tools be developed to address and integrate multi-material and geometric information into the functional design and manufacturing process?
- How can the overall data collected during the in situ measurements be used for design iteration, analysis inputs, optimization, quality assessments, and post-product delivery?

PROCESS MODELING AND DIAGNOSTIC CONSIDERATIONS

Ade Makinde, GE Global Research Center

Ade Makinde began with an overview of AM at GE. He explained that different laser processes are in use internally, including powder bed (i.e., DMLM and E-BEAM), wire-fed, and powder-fed, and materials being examined include alloys (Al-, Fe-, Co-, Ni-, Ti, etc.), refractory metals, ceramics, and polymers. GE has an AM development center for aviation—with a high volume AM facility that produces thousands of parts per year—and a corporate facility to drive innovation and implementation of advanced manufacturing technologies across the organization.

Process development, Makinde noted, depends on many different considerations with respect to materials, design, process machines, process planning, heat treatment, and post-processing. These factors are described below, and he cautioned that each of these factors contain uncertainties that need to be understood to avoid propagation throughout the whole system.

- *Materials.* The mean particle size, particle size distribution, morphology, composition, porosity, flowability, packing density, and material properties are all important to consider for the powder.
- *Design.* Design constraints exist such as operating and tolerance requirements as well as feature resolution and geometry.
- *Process machines.* AM machines also have their own specifications such as the laser type (e.g., wavelength, power), laser spot size and

variation, atmosphere and inert gas flow rate, preheat temperature and uniformity, humidity, material delivery, layer uniformity, residual stress build-up, and powder handling and reuse.
- *Process planning.* The process planning specifications include part orientation, path planning, build preparation, scan-paths factors (e.g., pattern, power, velocity, and layer thickness), support structure generation, and others imposed by the operator.
- *Heat treatment.* There are also metallurgy considerations during heat treatment including the as-built microstructure, temperature, ramp rate, phase formation, hold time, and atmosphere.
- *Post-processing.* Post-processing to achieve a defined surface finish depends on the process method, final surface finish, material composition, feature fidelity, tolerances, and hot isostatic press.

He highlighted some process issues such as rough edges and sagging on overhangs and particles being ejected from the desired area. Several types of sensors are needed to probe the AM process for errors: high resolution cameras and enhanced sensing for the melt pool, temperature, humidity and moisture, gas flow, and vibration, as well as methods to look into the powder bed, stress cracking detection, and packing density. While there have been several advances over recent years—including improved control of thermal lensing and the melt pool, enhanced information about the melt pool and powder bed, improved powder delivery, and decreased cost of implementation of in situ systems—Makinde highlighted the following in situ and diagnostics challenges in AM:

- High data rate collection is needed,
- Very large data sets need efficient and fast data reduction algorithms,
- Lack of sensors exist to capture the melting process in real time,
- High solidification rate (greater than 100,000 K/s) thermodynamic database does not exist for microstructure modeling,
- Non-uniformity of environmental conditions exists across the build chamber,
- Lack of access to machine process control information, and
- Large area with localized high temperature spots exists, which is a challenge for infrared measurement systems.

Makinde discussed some experimental methods for in situ monitoring that are being used, including photodiodes to see variation in melt pool size and geometry, high-speed imaging of the melt pool, and a closed-loop control interface monitoring module integrated with laser signals. Ultrasound is also used but he explained that porosity and cracking detection in a noisy environment pose challenges. Similarly, infrared and pyrometer can be used but thermography of a large area with localized hot zones is difficult. He also mentioned that high energy X-rays are used in research for fundamental process understanding but are not currently practical in industry production.

Integration of uncertainty analysis into process monitoring and diagnostics is important. Makinde noted that variability in surrounding conditions (e.g., heat transfer, laser spot size, and thermal lensing) across the build plate and during the build affects the part and deterministic modeling is insufficient. Powder packing varies from machine to machine (e.g., differences in re-coater, speed), as do thermal properties such as absorptivity and conductivity. Powder reuse would also make a large impact on AM viability in industry, he emphasized. He said a Bayesian hierarchical model (BHM) coupled with detailed physics-based models of melt pool is needed to compute and manage variability.

In situ measurements for design iteration, inputs, optimization, and quality can be validated with a high-fidelity physics model and then BHM can be used to manage and control variability for integration into design practices. This could improve the estimates of part life and the understanding of the interaction between the different stages of the process (e.g., powder size and distribution, laser, process parameters, part orientation, support structure, material properties such as surface tension and viscosity, surface finish, distortion and residual stress, and microstructure). He concluded by emphasizing that BHM could be used to develop fast, reduced-order models incorporating new build and legacy data to update the uncertainty models for use in real-time computations with integration into process monitoring.

BARRIERS TO WIDESPREAD ADDITIVE MANUFACTURING

Joseph Beaman, University of Texas at Austin

Joseph Beaman explained that the original goal of AM was to go directly from a CAD model to part manufacturing, avoiding the usual part-specific tooling and human intervention. He and his collaborators pioneered voxel manufacturing, or layered manufacturing, to make parts more quickly without fixtures or supports. They approached this by building machines that use a powder bed to support the structure implicitly. He commented that there are several market differentiations that fall within the umbrella of AM, and each balances strength and accuracy differently:

- Concept models, where form and fit are important but strength is not essential (e.g., architectural models);
- Patterns, where accuracy is essential and surface finish is important but strength requirements are low (e.g., casting applications);
- Machining forms, where strength is essential but accuracy is less essential because the part will be machined after it is built;[1]
- Prototyping, which aims to balance moderate accuracy and moderate strength to achieve a durable snap-fit part; and
- Manufacturing, which achieves high strength and high accuracy, is the ultimate goal of AM.

To get to widespread manufacturing, Beaman noted that several barriers need to be overcome, including those related to surface finish, production speed, cost of machines and materials, variation from part to part (mostly due to inadequate process control), and materials availability.

Several AM processes were discussed. The first process he introduced was stereolithography, which is a photopolymer process useful for patterns because the liquid process results in a smooth surface finish. The fused deposition modeling process currently dominates the hobby market. Inkjet systems can be good for patterns with limited applications for structural parts. He explained that the laser deposition process has many potential applications (e.g., multiple materials) but can be prohibitively expensive.

Process control is currently limited to nylon polymer structures because they can be processed without support structures. Beaman gave a quick overview of the history of selective laser sintering (SLS) thermal process control for direct polymer laser sintering (DPLS). In 1990, the process was to use a thermocouple temperature sensor in the part bed in conjunction with heaters in the part bed and the feed. Within a couple years, an infrared sensor on the part bed replaced the thermocouple sensor and made the process much easier to control. By 1994, three infrared sensors were being

[1] Beaman noted that these have an advantage over conventional production in that less machining is required, and therefore less material is wasted. However, the machining process can still be time consuming.

used, including two in the feed cylinders and one on the part bed, which allowed for warm-up and cool-down profiles to be developed. By 2001, control was further improved by employing infrared sensor drift correction, a physical flapper to control convective currents, and heater spatial variation correction. In 2004, multi-zone heaters and door sealing were utilized. The commercial SLS thermal process control for direct metals has no thermal control, Beaman explained. Instead, structures are built on a plate using support structures to help control thermal warping. Heat treatment is used to anneal parts with support structures and then the supports are then machined off, and the parts are machine finished. He commented that even though the process is complicated, it can still make complex shapes that cannot be made any other way.

He highlighted two main challenges in manufacturing: the necessary certification of SLS as a manufacturing process and the repeatability of geometry and properties. Improved process control for AM is required for the manufacturing market, Beaman commented. He emphasized that small production lots are often high value but every part needs to be precise and reliable without the advantage of learning on the part. He argued that process control is the biggest roadblock to using SLS but improving it is not an easy problem because the measurement environment is noisy with uncertain control actuation, and the time-temperature window required to process desired materials can be very tight.

Beaman highlighted three enabling technologies for small lot process control today, including advances in high-fidelity multiphysics computer models; advances in modern, nonlinear estimation and prediction; and inexpensive parallel computing. He also commented that modern Bayesian estimation methods can give predictions of the states of the system with characterized uncertainties. He explained that this is a two-step estimation process. The first is to propagate probability density function in real time from the physics-based model starting at t_1 and the second is to take a measurement at time t_2 and update probability. The difficult part is that probability propagation and Kalman filters are typically used for linear problems, while Monte Carlo is used for nonlinear problems.

Beaman and others are currently developing a laboratory scale system for process control test bed called LAMPS. This is a high temperature polymer system (approximately 350°C) with in situ measurement, open architecture software, and multiple new measurements and control inputs.

In conclusion, Beaman emphasized that the opportunity for layer-by-layer process control (both measurement and analysis in real time) is unique to AM. He stressed that small lots require new types of process control, including multiple measurements and real-time multiple physics. He stated that AM systems will be changing and newer methods will emerge, but AM is more complicated than most existing manufacturing processes. He cautioned that instituting standards at this point could limit innovation. Lastly, he stated that the cool down is important and should not be overlooked.

DIRECTED ENERGY DEPOSITION AND ELECTROSPINNING

Jian Cao, Northwestern University

Jian Cao began with an overview of directed energy deposition (DED), where powder is fed into a laser path with shielding gas. She highlighted three industrial applications of DED. The first is hybrid additive and subtractive machining used to make prototypes and small series production of complex lightweight and integral parts (e.g., for die and mold, aerospace, automotive, and medical applications). In this application, the flexibility of AM is combined with the precision of the cutting technology, making this process attractive to industry. She explained that a part can be built up in several steps and intermediate machining operations are possible. This hybrid process can achieve large and complex parts. The second application is the repair of worn medical, die and mold, and aerospace (e.g., blade tip) components. The third application is for corrosion and wear-resistant coatings on mold making, offshore drilling, machine tool, and medical parts.

Process parameters affect the quality of the final part, including powder deposition parameters (e.g., powder flow rate, shield gas flow rate, nozzle type, and powder shape, size, and type), laser parameters (e.g., laser spot size, scanning speed, power, and type), geometric parameters (e.g., hatch spacing, layer height, and build geometry and strategy), and substrate parameters (e.g., substrate surface condition, temperature, and size). She gave a few examples of how these parameters can impact results. If the powder flow rate is too low, the excess energy melts the substrate; if it is too high, the bond between layers can be weak (Imran, Masood, and Brandt, 2010). If the shielding gas flow rate is too low, oxidation occurs. If the laser power is too low, the powder will not sufficiently melt and porosity develops (Zhong et al., 2015; Imran, Masood, and Brandt, 2010). On the other hand, if the laser power is too high, trapped gas can lead to another type of porosity (Wolff et al., 2016). Changing the laser type and the corresponding wavelengths (e.g., from an infrared laser to blue laser) can potentially greatly improve the absorption of laser energy and improve precision.[2] However, the cost of the new lasers can be a factor. The scan speed and laser power can affect the underlying microstructure (Kobryn, Moore, and Semiatin, 2000). Different build geometries can also impact porosity (Susan et al., 2006) and deposition direction can impact the microstructure (F. Liu et al., 2011).

Cao mentioned several sensing and characterization methods. Two approaches toward real-time melt pool sensing use either imaging with infrared and visible-wavelength cameras or emission detection with variations of optical pyrometry or spectroscopy (Dunsky, 2014) or acoustic wave (Sherman, Liou, and Balogun, 2015). Two powder delivery rate sensing methods discussed by Cao utilize either an electronic scale to measure the change of weight of metal powders in the hopper or an optoelectronic sensor to decrease laser energy when the powder delivery rate is increased (Hu and Kovacevic, 2003). Techniques to use laser ultrasonics to detect porosity are also being developed (Slotwinski, Garboczi, and Hebenstreit, 2014). In situ X-ray diffraction is being used on rapidly heated and cooled Ti alloys to examine crystallographic phases (Leinenbach, 2015). Neutron diffraction can penetrate deeply into a part and can be used to measure stress (Hoye et al., 2014). A novel submicron X-ray microscopy can be used for subsurface imaging and reveals three-dimensional microstructure (Lavery et al., 2015). Cao noted that process control is difficult but there are ongoing efforts in powder flow control (Tang et al., 2008), layer height control (Song et al., 2012), and heat input control (Mazumder, 2015) that may help.

Cao also gave an overview of the electrospinning process, as shown in Figure 4-1, where a high voltage is applied to the nozzle and plate collector, resulting in far-field electrospinning when the nozzle is far from the plate. This achieves fast deposition of microfibers and nanofibers. When the nozzle is close to the plate, near-field electrospinning takes a random deposition process and converts it into a controlled AM process. She emphasized that electrospinning has unique in situ monitoring requirements due to printing via continuous nanofiber and microfiber deposition. The system typically operates using open-loop control, and metrology and characterization are typically done after deposition via a scanning electron microscope. Process parameters for electrospinning include electric field strength, flow rate, deposition speed, and evaporation rate. She explained that the online diagnostic requires high magnification and high temporal resolution of

[2] Nuburu, Inc., for example, makes a high-power and affordable blue laser that could potentially be used for AM.

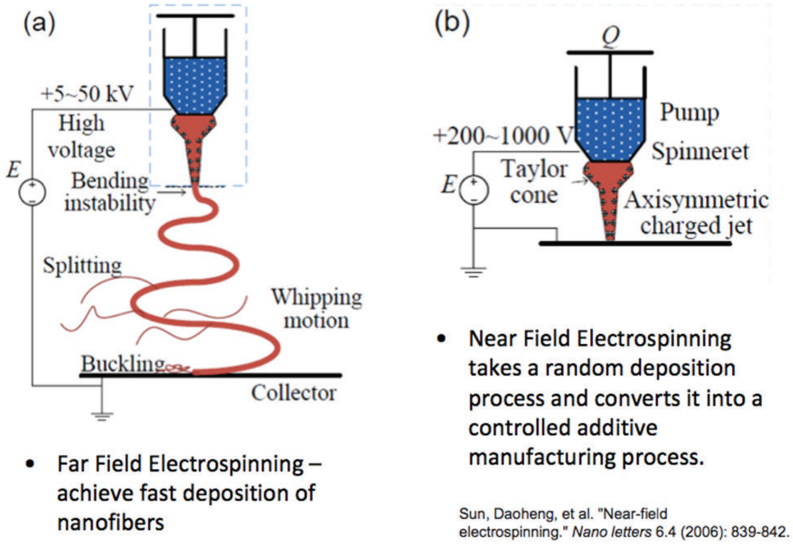

FIGURE 4-1 Electrospinning process with (a) near-field spinning and (b) far-field spinning. SOURCE: Jian Cao, Northwestern University, presentation of Martinez-Prieto et al. (2015) to the workshop.

the deposition process over large areas as the fiber diameters range from approximately 5 nm to tens of microns and the collector speeds range up to hundreds of millimeters per second, with areas of tens of centimeters. The monitoring of the fiber in flight aims to track the diameter, speed, and orientation (Kim et al., 2010; Huang et al., 2003). This monitoring can be a challenge. She noted that current in situ sensing is limited to environmental control (e.g., humidity, temperature), electrical current, and limited optical feedback (D.L. Liu et al., 2011; Samatham and Kim, 2006).

There are several applications of electrospinning, including three-dimensional cell scaffolds for cell growth and drug testing (developed by Electrospinning Company), air filters and battery separators (developed by Elmarco), and AVflo™ vascular access grafts with multilayer structure (developed by Nicast). Cao explained that electrospinning can also be used to produce copper nanofiber webs for use with flexible electronics; their high fiber density leads to resistance reduction, high transparency, and conductivity (Wu et al., 2010; Hochleitner et al., 2015; Zheng et al., 2010; Wang et al., 2012). Efforts are underway to increase process control (Martinez-Prieto et al., 2015). Results show increased repeatability in deposition and increased fiber deposition control when the secondary electrode is used. Other efforts include the proposed stationary electrode ring designs, with either one or four independent potentials, and the electrospray-assisted Langmuir-Blodgett assembly (Nie et al., 2015) to help prevent particle aggregation.

With respect to research needs, Cao commented that more advanced digitally-compatible computational design tools are needed to integrate multi-material and geometric information into the design of manufacturing processes considering uncertainties. She emphasized that many of the limitations of AM can be addressed with predictive simulation paired with equipment innovation, effective process control, and a strong understanding of the processes, materials, and properties involved. In concluding, she acknowledged her funders[3] and collaborators[4] in these areas.

Discussion

Following their presentations, Ade Makinde, Joseph Beaman, and Jian Cao participated in a panel discussion moderated by Anthony DeCarmine from Oxford Performance Materials. An audience member began by elaborating on the case study Joe Bishop of Sandia National Laboratories presented on the AM titanium preform. He noted that the company that built the AM machine went out of business in part because it lacked process feedback control and process monitoring. It was a gravity-fed powder process with a CO_2 laser that resulted in a significant amount of unfused powder particles, and the AM part required substantial machining. This experience led researchers to collaborate in the development of e-beam wire-fed AM with closed-loop process feedback control.

A national laboratory participant suggested two ways to add computational power to the feedback loop. The first is taking a lesson from tomography machines by integrating GPU and other processors into the machines. The second approach is to utilize commercially-available cloud computing on networked machines. Makinde agreed that cloud computing has a lot of potential in this area. Bishop wondered if cloud-based systems are a practical real-time approach and if data security is a concern. The

[3] Sponsors include NIST, NSF, DOD, and DMG MORI.

[4] Collaborators include Sarah Wolff, Jacob Lee Smith, Jennifer Lynn Bennett, Fuyao Yan, David Pritchet, Hong-Cin Liou, Nicolas Camilo Martinez Prieto, Ebot Etchu Ndip-Agbor, Zequn Wang, Oluwaseyi Balogun, Wei Chen, Kornel Ehmann, Jiaxing Huang, Greg Olson, Wing K. Liu, Federico Sciammarella, Joseph Santner, and Eric J. Faierson.

participant commented that most of the major cloud computing companies have comprehensive security considerations that may alleviate security concerns and that real-time is approachable, with a potentially higher cost to avoid long wait times.

A participant asked about the effect of vibration sensitivity on part quality. Makinde said that vibration is an issue that has not been sufficiently addressed; he stated that many of the machines available today will only work for prototype applications because industrial applications demand more reliability. Bishop also agreed this is a concern. Cao commented that, to combat this issue, the machine she and her collaborators are building rests on a granite table to significantly reduce vibration impact. An online participant noted that the U.S. Navy attempted to use AM onboard ships but struggled to overcome vibration and machine motion.

An online participant noted that powder-bed processes seem to work well for single-metal AM but wondered how these processes could adapt to the realm of multiple materials. Bishop responded that multiple materials are perhaps too challenging in a powder bed; he believes multi-materials parts will have to be constructed using a deposition process.

A participant wondered about which sources of variability the AM community should be concerned. Bishop and Makinde commented that multiple machine variability is challenging and approaches to minimize it are being pursued actively in industry, including approaches to account for variability in the design process. Cao noted that laser and sensor degradation are contributors to the variation. She suggested that translating functional metrology to AM to combine simulation and experimental data could offer a future approach to part qualification and certification, given potential variation. Another participant asked if it is possible to create standards for machines, control, or process to help improve variability. Bishop said that standards could be created for geometries with specific materials, assuming there are agreed-upon ways to measure compliance, and this could be useful to advance machine manufacturing. Makinde agreed that standards in conjunction with the machine calibration already done could help. Cao emphasized that it is important for users to understand machine idiosyncrasies and learn to calibrate accordingly.

A participant asked about part aging and if there are approaches to sample and monitor parts after they have been produced (e.g., integrating diagnostics into the monitoring). Makinde stated that for metal parts, the as-built microstructure is usually not preferable so the part is then put through a heat treatment to achieve a desired microstructure. Phase fields are used to understand the thermocycles that need to be implemented. A HIP treatment is also often done to address porosity. Bishop noted that data from the various phases of development could be stored to create a digital thread of each layer of a part to then compare with experimental testing. Makinde said these data are often compared to explore potential areas of concern. This can create a solid understanding of how the part will work now but the technology is not available to reliably reproduce the part on a different machine at a different time.

A participant asked about how to mitigate crack formation when utilizing laser powder-bed diffusion at the lower temperatures at which machines typically work (below 500°C). Bishop responded that the base plate can be heated (up to 400°C), but it is difficult and expensive to heat uniformly higher than that. In response to another question about technical advantages needed to build better metal parts, Bishop said that better thermal control is needed to build with fewer support structures and base plates.

A participant from a national laboratory asked Bishop if there is a way to go back to previous voxel efforts to design with uncertainty. Cao commented that this is being explored. Wing Kam Liu agreed, noting that voxel efforts for CAD are utilized but performing the conforming mesh simulation can be prohibitive.

An audience member asked a question about monitoring and calibration: If this is done layer-by-layer, is there a minimum number of layers that has to be calibrated to control quality? How can the resulting data be used for predictive or monitoring purposes? Bishop noted that when many parts are built, one part could be used for calibration without much marginal expense. He suggested that modeling could be used to extrapolate findings from one part to a different geometry. Makinde stated that the emphasis needs to be on the entire process development to determine the correct parameter set for a specific build. He said the data coming out of the process is substantial and difficult to handle and use. Cao said that numerical models rely on design parameters that can be tweaked and it is difficult to make these parameters universal; improvements will come from a better understanding of the underlying physics and the sensors used to capture information. Makinde suggested that Bayesian analyses can be used to incorporate information from past processes to improve future processes.

A participant asked about metal powder recycling and the point at which reuse becomes problematic. Makinde acknowledged this has been studied by some researchers. Bishop said that reuse is often approached by mixing reused powder with new powder.

ENHANCING END-USER CONTROL

David M. Keicher, Sandia National Laboratories

David M. Keicher explained that he and his collaborators[5] are looking at how to approach AM differently to improve the experience of the end users. There are a number of unique AM machines and each uses unique black-box software. He highlighted some challenges in AM, including a lack of confidence in the integrity of AM parts, the need to accelerate integration of model-based processing into AM, user-unfriendly equipment, closed architecture of machines, and variations in feed stocks. AM-specific diagnostics challenges include detecting occurrence of build defects, providing a metric for quality control, controlling dimensional accuracy, and enabling platform-independent printing. He emphasized that a combination of process and system diagnostics is needed.

Some examples of potential diagnostics were given. The first possibility was real-time spatially-resolved defect and geometry detection. This can be an open-loop process with data collection and analysis for quality control or a closed-loop process with data collection and analysis for real-time control. Another possibility he mentioned is to use system diagnostics for process transfer, including beam spot size measurements, laser power measurements, and state-of-health monitors (i.e., optics). He discussed a closed-loop process control with the LENS system, explaining that the closed-loop process control enables process consistency but does not move away from empirically-based process development. He also mentioned model results for melt pool control where process modeling is able to replicate real-world behavior of the melt pool with and without closed-loop process control.

Prior LENS research, Keicher explained, has focused on graded composition demonstration and process characterization modeling (e.g., a part heats up during the build and the heat flow changes, resulting in different microstructures and properties across the part) using a variety of LENS metals (e.g., Ti-6Al-4AV, Aeromet 100, stainless 304L and 316L, tool steels, Inconel, and graded NiTi). He emphasized that this approach has a number of advantages but questioned why it is not being used more heavily.

He explained that the current approach to AM disconnects the theoretical and experimental capabilities (e.g., predictive modeling, process knowledge, and diagnostic results) from the end-user application (e.g., process,

[5] Adam Cook, Josh Sugar, Daryll Dagel, Grant Grosseetete, Lauren Beghini, and Arthur Brown.

qualification, reliability, and product assurance). Efforts in both areas are important and opportunities exist to leverage developments in each area to accelerate adoption of AM. Tools are needed to bridge this gap. He highlighted validation as a means to connect and accelerate new process development, noting that model-based experiments lead to new process development for new materials and multi-materials, and fewer experiments are needed to support new process validation.

The traditional manufacturing approach using CAD and computer-aided manufacturing (CAM) is to capture design and material knowledge in the CAD implementation (e.g., three-dimensional modeling, simulation, and design optimization). This information is then transferred to the CAM process, capturing machine process knowledge through toolpath generation, tool selection, and speeds and feeds. The end product is the finished part. This can be done using only a separate CAD post processor and is independent of which CAM system machine is used.

According to Keicher, the goal is model-based feedforward control to provide a path for end users to leverage predictive capabilities to accelerate development in AM. To facilitate this, a process simulator would take the predictive AM CAD modeling—with the corresponding microstructural modeling, thermal and residual stress modeling, multi-material modeling, and multiphysics-based topological optimization—and translate the results into a geometry for the model-based feedforward control tool. This tool generates the toolpaths and embeds controls to validate simulation results. These simulation results can then be iterated with the process simulation (and revised as needed) until the part is made. This part can then be validated to qualify process and parts. He expects that this process could be applied to most of the AM approaches currently used.

The approach for generating toolpaths with embedded toolpath commands is similar to the process for conventional manufacturing. Keicher explained that the part is sliced into layers and toolpath vectors are drawn through each layer. Process conditions need to change as the toolpath approaches a discontinuity to ensure desired behavior throughout the part. Combining process controls with toolpath vectors could create a contour map for smart toolpaths, and this approach could be used for a variety of AM techniques.

To conclude, Keicher described several benefits of integrating CAD and CAM approaches for AM. The first is increased confidence in the integrity of AM parts. Predictive modeling results can be used to generate toolpaths to drive processes, and part properties can also be correlated to predicted properties. This improved process confidence can lead to a streamlined development and manufacturing as well as enhanced component design space. Another benefit is the accelerated integration of AM model-based processing. He emphasized that there are significant opportunities to advance validity in AM, demonstrate a leadership role in providing certainty in AM, and improve virtual prototyping speed in process development. A third benefit discussed related to improving usability for otherwise user-unfriendly equipment. This approach can provide process knowledge to overcome steep learning curves, and post processors can provide vendor-specific commands to a broad range of equipment. The fourth benefit discussed related to the closed architecture of AM machines. Post processors can adjust for machine differences and provide users with edit capability to enable open-architecture systems. The last benefit discussed related to variations in feedstock properties. He emphasized that model-based prediction can account for feedstock variability, and predictive capabilities accelerate with elemental blending of materials and development of gradient structures.

ANALYSIS OF HIGHLY CORRELATED DATA SETS TO ESTABLISH PROCESSING-STRUCTURE-PROPERTY RELATIONSHIPS FOR ADDITIVELY-MANUFACTURED METALS

Edwin Schwalbach, Air Force Research Laboratory

Edwin Schwalbach began by discussing the potential benefits and challenges of AM. Near-term benefits include short lead time and little tooling required, which makes small lot production possible. In the long term, AM can make complex shapes, graded or tailored structure and properties, and hybrid structures not possible via conventional processing. However, there is currently an undeveloped understanding of the links among processing, structure, and property due to process complexity, he explained. The design rules and process specs are lacking or nonexistent. He noted that AM complexity necessitates an integrated computational material science and engineering approach to address challenges, both temporal (e.g., complex energy input and resulting thermal history) and spatial (e.g., wide range of scales, complex build can easily have 10 km of track). He and his collaborators[6] are working to develop a research vision with three steps:

[6] Collaborators include Michael Groeber at the Air Force Research Laboratory, and Ryan Dehoff and Vincent Paquit at Oak Ridge National Laboratory.

1. *Collecting and generating pedigreed process data to capture an accurate and complete description of the process.* These data are typically divided into planning and execution data. Planning data relates to the processing intent and includes part geometry from CAD models and process condition maps. Execution data relates to the processing reality, including log files, infrared videos, thermal histories, and in situ imaging for porosity. He noted that both qualitative and quantitative data are useful.
2. *Conducting an advanced material characterization to describe process outcome.* This includes non-destructive characterization (e.g., ultrasound and ray) and destructive characterization (e.g., conventional microscopy and serial sectioning).
3. *Reducing the data from terabytes of data and conducting data analysis to uncover actionable information.* This involves combining and registering the planning, execution, and characterization of data sets and model outputs to establish correlations in properties and zone parts based on processing conditions. Some challenges include the range of data modalities, disparate spatial and temporal scales, and large data sets (e.g., 1 TB per build). He noted that he and his collaborators have been utilizing SIMPL[7] (an open-source software library for dynamic, hierarchical management of spatial data) and DREAM.3D[8] (an extensive tool suite for analytics of the internal state of materials, built on SIMPL). He emphasized that this infrastructure is useful for other materials problems.

Schwalbach illustrated this framework with a data fusion example using a Ti-6Al-4V cylinder with an intentional pore in the center. They used X-ray CT scans to examine the porosity, the log file to examine the execution and process anomaly, and parameter maps to examine the planning and parameter changes. These data were manually compiled with melt current data to better understand the pore volume fraction and average current throughout the cylinder.

In conclusion, he emphasized that more integrated computational material science and engineering tools are needed for digital data management for AM. These tools would help in the efforts to establish

[7] The website for SIMPL is https://github.com/BlueQuartzSoftware/SIMPL, accessed August 18, 2016.

[8] The website for DREAM.3D is http://dream3d.bluequartz.net//, accessed August 18, 2016.

process-structure-property links to enable AM design and provide digital data to address process specification challenges.

IN-PROCESS SENSING OF LASER POWDER-BED FUSION ADDITIVE MANUFACTURING

Yu-Ping Yang, EWI

Yu-Ping Yang explained that in-process sensing of laser powder-bed fusion AM is necessary and is being studied collaboratively by researchers at several organizations.[9] Conventional material production steps are tightly monitored and controlled to ensure quality, he explained. In contrast, AM is merging materials creation directly into a functional part. Laser powder-bed fusion systems do not possess the same level of quality monitoring that conventional manufacturing systems employ so in-process monitoring is necessary to improve reliability. He explained that each weld is an opportunity for a defect and without process sensing, part developers must rely on process development and post-process inspection. However, post-processing inspection can be too difficult and costly. The incremental approach to material creation allows defects to be sensed as they are created while also accessing difficult-to-inspect areas. If a flaw is detected (e.g., process deviations, geometry, distortion, bed flatness, metallurgical, pores, lack of fusion, and cracking), long builds can be cancelled and restarted, therefore saving time and resources. Advanced sensing could also lead to advances in control, he stated, as more information is known about local and global material and process iterations before, during, and after the part is built.

He described several facets of this technical approach. Yang noted that it is difficult to install sensors in commercial machines so he and his collaborators first developed a laser powder-bed fusion test bed to allow for sensor evaluation without physical or software constraints. He described some of the hardware considerations, including checking positional axes to be within 10 micron resolution, determining laser focus and power calibration, and completing build platform leveling. There were also several control

[9] Collaborators include EWI (Shawn Kelly, Mahdi Jamshidinia, Jake Marchal, Paul Boulware, Connie Reichert, Greg Firestone, and Lance Cronley), University of North Carolina at Charlotte (John Zeigert, Angela Davies, Kyle Zhang, and Will Land), Georgia Institute of Technology (Jaydeep Karandikar, Masouhmeh Aminzadeh, and Thomas Kurfess), Paramount Industries Inc. (Jim Williams), B6 Sigma Inc. (Mark Cola and Matias Roybal), Stratonics (Jim Craig), EOS, and GE Aviation.

decisions, including setting up one computer for sensor test control and another for sensor data acquisition and display, and integrating all motor drives, solenoids, computers, sensors, power, and other components into the control cabinet. Local and global sensors were also installed to monitor the area near the point of material fusion and defect occurrence over the entire bed, respectively. Test sensors can be used to produce thermal and optical images. He explained that an advantage of this approach is the open architecture system, which allows for complete control over toolpath generation (so far restricted to simple shapes), laser power, travel speed, and position of beam. The position of the beam can be tracked to link with sensor data, and users have open access to the beam delivery path.

Local and global sensors can be set up by first integrating sensors into the test bed, then developing the defect-generating build matrix, Yang explained. The sensors can then be evaluated across the build matrix to enhance sensor quality signals. Local sensors (e.g., photodetector, spectrometer, high speed video, two-color optical, and pyrometer) can be used to view the process at the point of fusion and to collect information at and surrounding the melt pool. Global sensors (e.g., high resolution imaging, laser line scan, and global thermal) collect information before, during, and after a layer is scanned. Table 4-1 details the types of defects that can be identified from some local and global sensors.

Improved sensing in conjunction with experimental measurements can help validate numerical models. He elaborated that computational fluid dynamics can be used to predict the fluid flow in the melt pool and optical images can be used to validate their predictions to improve the fundamental understanding of the AM process. Similarly, thermal models used to predict temperature distributions can be validated using thermal images (Jamshidinia, Kong, and Kovacevic, 2013). Sensing can also help validate mechanical models for temperature, stress, and deformation.

Both local and global sensors are evolving, Yang stated. Local sensors are currently collecting data at approximately 10 percent of the desired rate (or once every 10 melt pools). Thermal characteristics can be explored using high-resolution imaging of the melt pool, which currently operates in single-color mode due to software issues. Visual information can be gathered with high-speed video, balancing illumination and focus issues. Spectrometers have slow response times, overall intensity dependencies, and limited analysis of line sensitivity. He noted that photodetectors could prove useful if spectral lines can be related to defects. Global sensors are capable of collecting data at every layer. Global thermal sensors are showing

TABLE 4-1 Sensor and Defect Type

Process Observation	Sensor	Defect Type					
		Process Deviation	Distortion	Geometry	Bed Flatness	Metallurgical	Volumetric Defects
Local	High Speed Video	Defect Generation Understanding					
	Thermal Imaging					X	X
	High Resolution Imaging		X	X	X		
Global	Laser Line Scanner		X	X	X		
	Thermal Imaging					X	X
	Photogrammetry (UNCC)		X	X			
	Projection Moiré (UNCC)		X	X	X		

SOURCE: Yu-Ping Yang, EWI, presentation to the workshop.

promising results, he noted. Large embedded defects can be seen clearly but may be masked when overhangs are present. Machine vision and laser line scanners are also promising but are algorithm dependent. There are still some technical gaps to be overcome, especially in the area of evaluating sensor effectiveness. He noted big data poses a substantial challenge in terms of dealing with throughput, processing and distillation, and storage.

In conclusion, he emphasized that there is more to AM than the process and it should be treated like any other manufacturing system. Quality control and in-process sensing will be necessary to advance AM. He reiterated that there is a unique opportunity with in-process sensing to inspect layer by layer.

Discussion

Following their individual presentations, David M. Keicher, Edwin Schwalbach, and Yu-Ping Yang participated in a panel discussion moderated by Slade Gardner from Lockheed Martin Space Systems Company. A participant asked if the panelists have advice on statistical approaches for selecting extreme values, spikes, or rare events in sensor data to better identify defects. Yang responded that EWI is developing the use of a passive sensor to monitor sound within the test bed and detect unusual noises that may indicate a potential defect. Schwalbach agreed that better rare event identification techniques are needed because the current approach of collecting all data is becoming difficult to manage.

A participant commented that results of computational models should not depend on coordinate systems and asked how this can be achieved for AM given that it has many coordinate-dependent operations (e.g., the orientation of the part when it is sliced for analysis, the path the laser travels). Keicher replied that the layering effect can be minimized by modifying the process parameters in a way that increases the grain growth across the deposition layer. Also, doing a HIP treatment can further increase material homogenization. Schwalbach noted that orienting a part to reduce the effect of geometry has become an art but is not systematically conveyed. He mentioned that there is a potential in the future to use materials systems that are less sensitive to geometric orientation or can easily be remedied with post processing. A participant asked Yang if the melt pool monitoring technique to determine delamination can account for porosity. Yang said that the goal is to detect 10 micron pores but EWI is not able to do this yet.

Gardner asked about CAD and CAM for path planning. He noted that CAD models can become very sophisticated and can contain a significant amount of information per volume element (e.g., material properties, vendor source properties), and he wondered if there is a corollary mechanism to pass information in CAM for path planning. Keicher noted that offset surfaces can be put into CAD models to embed information into the geometry. The contour maps represent different processes and intersecting these with the toolpath generator results in the embedded process control toolpath commands. He said this is still conceptual but inserting the offset surfaces into a CAD model should not be too complicated. Gardner asked if in situ diagnostics and sensing can be brought into the process and if software exist to collect these data according to the CAD instructions to record the position. Keicher said they are currently capturing thermal data to correlate with positional data about the system. He said that these efforts are in the beginning phases and additional software would be helpful. Schwalbach added that some groups are working to develop tools but none are commercially available yet.

Gardner noted that the diagnostics and sensing described in this session relate to powder-bed AM processes; he asked if there are other in situ approaches for different AM processes. An audience member commented that multiple materials are used within polymer AM, and work is being done to characterize the local chemical composition. Schwalbach said that some of the talks in this session discussed tools to examine graded chemistry and microstructures *after* a build is complete, but tools to examine this *during* a build are not readily available. Keicher commented that Sandia is working to incorporate a suite of sensors into the process to improve capabilities.

Gardner asked about limitations of sensors and whether advances are needed in sensor technology. Yang said it is currently difficult to measure stress dynamically. An audience member added that almost all the properties needed to assess stress can be measured, though not quickly enough with the low-intensity X-rays. Schwalbach commented that techniques to look deeper into a part (as opposed to just the surface) would be helpful. Keicher said that work is being done to collect data on a block of material to compare with parts made of similar material. This can be used to check part measurements. Schwalbach said the complicated AM geometry may necessitate after-build inspection. The audience member commented that X-ray CTs are being used but they do not provide traceability for quantitative metrology.

5

Additive Manufacturing Scalability, Implementation, Readiness, and Transition

The fourth sessions of the workshop discussed additive manufacturing (AM) scalability, implementation, readiness, and transition. This includes fundamental bridges that must be forged to take analytical, computational, and mechanistic models and initial laboratory experiments into pilot production lines, and subsequently into full-scale production for rate, quantity, and size, considering mass customization theme.

Yung C. Shin (Purdue University), Lyle E. Levine (National Institute of Standards and Technology), Anthony DeCarmine (Oxford Performance Materials), Rainer Hebert (University of Connecticut), Alonso Peralta-Duran (Honeywell International Inc.), and Tahany El-Wardany (United Technologies Research Center) discussed the following questions:

- What is the path for utilizing fundamental results for AM and scaling them for use in production?
- What are the roadblocks that hinder the scaling of AM technologies into production and use in systems?
- Do any of these roadblocks represent issues that can be best addressed through additional fundamental research?
- What are future applications, markets, and industry partners that may leverage the fundamental research and scale it into production?
- What measurements of quality or systems are appropriate that correlate computational and analytical methods to practical implementation?

- Which AM software architectures and databases can be used for AM model development?
- How can careful design of validation experiments for model validation, uncertainty quantification, and in situ process monitoring be incorporated?
- Can software be developed, integrated with precision engineering, and integrated into engineering work flow?
- Are there drivers to integrate computational simulation and advanced optimization methodologies to enable unique AM design?
- What opportunities exist for public-private partnerships to advance high-performance computing (HPC) capabilities for AM? How should these partnerships benefit from shared technological advancements?
- Do processing standards change with an analytical and mechanistic model approach to implementation of full-scale AM?

ADDITIVE MANUFACTING: CAPABILITIES, CHALLENGES, AND THE FUTURE

Yung C. Shin, Purdue University

Yung C. Shin began by emphasizing that the many AM processes—powder-bed fusion (e.g., SLS, EBM, DMLS), directed energy deposition (e.g., laser), material extrusion (e.g., FDM), vat photopolymerization (e.g., SLA, 2PP), binder jetting, material jetting (e.g., MJM), and sheet lamination (e.g., laminated object manufacturing, ultrasonic)—offer significant opportunities to embark on new frontiers of manufacturing. In addition to the capability of building three-dimensional functional parts from CAD drawings in one step, AM offers the opportunity to synthesize novel materials and gradient structures that cannot be made by conventional processes. He explained that AM processes can impart local properties as needed, thus offering new concepts of design, while allowing on-demand manufacturing without traditional inventory constraints. These processes can also provide individual customized products with little or no added cost and lead time.

However, he noted that there are lingering issues that must be resolved. The first is determining the path for utilizing fundamental results for AM and scaling them for use in productions. Another issue is the need to understand which roadblocks hinder the scaling of AM technologies into production and use in systems, as well as whether any of these roadblocks represent problems that can be best addressed through additional fundamental research. Also, he wondered about future applications, markets, and industry partners that may leverage the fundamental research and scale AM into production. He referenced the many facets that go into an AM workflow, including the geometry design, computational tools and interfaces development, material design, and process modeling and control tools. These complex factors are illustrated in Figure 5-1.

AM has many application areas, especially when combined with functional materials like the shape memory alloy Nitinol, which can be used in biomedical field applications to make orthopedic implants, medical stents, orthodontic wires, bone plates and screws, and surgical devices, Shin explained. It can also be used for aerospace applications such as sensors and actuators, as well as for other applications such as vibration dampers and vibration isolators. He stated that these materials can be made by mixing different powders to be used with directed energy deposition, applying a post-build heat treatment, and then formulating the application. This allows porosity and density control while creating a functionally-gradient material.

Bulk metallic glasses (BMGs) are one example he gave of new material synthesis. BMGs have a suppressed nucleation of crystalline phase atomic arrangement that results in superior properties (e.g., strength, hardness, wear, and corrosion resistance), according to Shin. BMGs combine high yield strength with elastic limit and have excellent resistance to wear and corrosion, but they have limited glass-forming ability, fracture toughness, and ductility and failure strain (Telford, 2004; Miller and Liaw, 2008). He noted that the material phase can also be controlled to have a partially-amorphous and partially-crystalline material to improve its ductility while retaining the advantageous features of BMG.

Another application area Shin described is the remanufacturing of gas turbine blades. These expensive parts are subjected to difficult operating conditions (e.g., temperature, velocity), and they often experience expedited erosion of the external protective barrier on the blades and increased vulnerability to abrasive effects of ingested particles. AM can be used as a cost-effective alternative to repair defective blades and improve performance.

Shin described several roadblocks that hinder the scaling of AM technologies into production and use in systems. Current design tools and material design capabilities for AM are inadequate, he stated. Also, different AM processes involve different materials and mechanics. He emphasized that the lack of accurate and reliable predictive computational tools is a problem, especially since these tools should be capable of predicting resultant

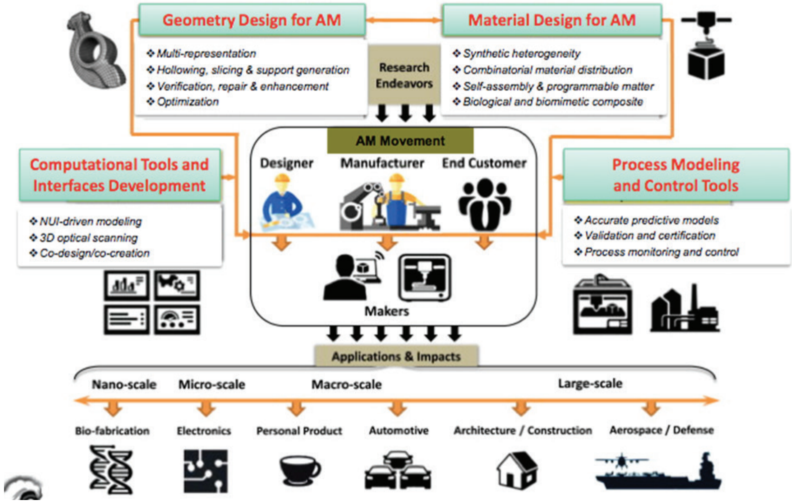

FIGURE 5-1 Additive manufacturing workflow. SOURCE: Yung C. Shin, Purdue University, presentation to the workshop, adapted from Gao et al. (2015).

microstructure, phase, density, form accuracy, finish, residual stresses, and other mechanical, chemical, and thermal properties. The lack of validation and certification standards (for physical and numerical results) and a mostly open-loop process control also pose challenges, as do the long build times that require the process throughput improvement.

Geometry design for AM is challenging. Shin explained that most CAD systems are currently based on boundary representations and tools for topology optimization with local material properties that are lacking. The use of a stereolithography (STL) file format is difficult because it does not fully support AM processes, he commented. In addition, it is difficult to design with multi-materials or by embedding foreign objects (e.g., hybrid processes).

He also described challenges with material design for AM. Current design practice is limited to the shape of the given material, and few material choices exist for AM. He explained that both complex structural design with optimized design performance and multi-material modeling for heterogeneous objects are needed.

Process modeling for AM is also challenging. For example, he noted that various AM processes involve different physical mechanisms and materials, making it difficult for a small group of researchers to have necessary expertise in all areas. AM processes require more process parameters than traditional manufacturing processes. Currently no simulation system exists that can be used directly by AM developers and users, Shin said. In addition, existing computational models are not suitable for iterative or real-time design since they are too intensive computationally and because AM research on process modeling is currently fragmented.

Multiscale modeling of laser-based AM processes is complex, involving material and laser inputs and modeling of heat and mass transport (e.g., laser–matter interaction, heating, cooling, melting, solidification, and evaporation). Changes such as solid-state phase transformation and dendrite growth must also be considered. Outputs of these types of analysis include system geometry and properties relating to the microstructure, material phase, strain, and stress. These analyses span multiple scales, from the atomistic scale (e.g., phases, compositions), to the microscale (e.g., microstructure, porosity), and to the macroscale (e.g., heat and mass transport in melt pool).

Trade-offs between model predictive capability and computational effort must be understood well and balanced effectively, Shin emphasized. The computationally intensive nature of these simulations can be addressed by increased parallelization or by reducing the complexity of the physics modeled. However, he cautioned that oversimplification of simulations can reduce model accuracy. By better utilizing multiscale modeling, such as atomistic modeling, to achieve critical material properties at various conditions, the challenge of doing material design and prediction capability with numerous simulations for optimization is eliminated.

The path for utilizing fundamental results for AM and scaling them for use in productions, Shin explained, relies on new design tools for AM. This includes multiscale design that connects the nanoscale, mesoscale, and macroscale. The high-dimensional volume or voxel-based approaches to represent complex geometries and multiple materials with process parameters embedded could be particularly helpful. He stressed that model validation and printability checking are crucial steps. Process validation models can be approached by taking an AM process simulator that outputs microstructure features, materials physics, phases, properties, and stress and strain distributions. These outputs are then used as inputs for a multiscale finite element solver. The finite element model then creates inputs for virtual experiments. He commented that topology optimization will likely be beneficial as well.

Scalability can also be improved by advancing research in material design for AM, Shin stated. An approach he mentioned is engineering material properties via combinatorial material distribution or microstructure control, including multi-material modeling and heterogeneous multifunctional design. Other important areas that should be advanced, he said, are the capabilities for functionally-gradient material, new material synthesis, self-assembly and programmable matter, and biological and biomimetic composites design.

He reiterated that process modeling, validation models, and monitoring and control for AM are important. It is necessary to develop a better understanding of the basic physics for various AM processes, for which multiscale modeling is needed. Mechanisms for longer-term collaborative efforts among researchers or between academia and industry to develop robust, accurate, and efficient process models for various AM processes should be established, he explained. This includes national level consortia for AM process modeling (that can be divided into process specific ones) and a repository or database for material selection, properties, or response surfaces. Shin argued that the community needs standards for certification and validation of AM processes, robust and reliable in-process monitoring, and closed-loop feedback control methods. Shared high-power (parallel processing) computational resources would also be helpful.

Shin discussed some future applications (e.g., high performance products with localized properties, geometric complexity, embedded sensors, electronics, and actuators) that may leverage the fundamental research and scale it into production. He also noted that AM holds potential in remanufacturing, multiscale products, customized products (e.g., implants and prostheses), tooling, fixtures, rapid prototyping, and education.

SOFTWARE ARCHITECTURE, DATABASE DEVELOPMENT, AND MODEL VALIDATION: TOWARDS A COMPUTATIONAL BENCHMARK IN ADDITIVE MANUFACTURING

Lyle E. Levine, National Institute of Standards and Technology

Lyle E. Levine opened his presentation discussing what measurements of quality or systems are appropriate that correlate computational and analytical methods to practical implementation. Conventional alloys, he explained, have many decades of experience and study, controlled composition and microstructure, known thermal and deformation history, and well-understood properties and failure behavior. Conventional manufacturing is viewed as having controlled dimensions and surface finish with relatively few material or build flaws. In contrast, AM alloys have uncontrolled microstructures (e.g., phases, grain sizes, texture), large stresses (both macro and micro), extreme compositional gradients, reproducibility issues, and build flaws. He emphasized that dimensional accuracy and precision depend on the geometry, macroscale stresses, and difficult features. The mechanical behavior of a final part (after any post-build processing) also depends on the microstructure and local stresses.

Software architecture and databases for AM model development were also discussed. Levine explained that micro-level build multiphysics simulations can feed into macro-level build simulations. The output from the macro simulation serves as inputs for both the macro residual stress simulations and the microstructure evolution models, both during and after the build. Micro residual stress simulations take inputs from the microstructure evolution models and produce outputs that inform material property predictions.

Careful experimental design for model validation, uncertainty quantification, and in situ process monitoring is important, Levine noted. In situ process monitoring, such as thermography, secondary laser probes, and in situ X-ray fluorescence and diffraction can all provide useful information. Thermography, he explained, can be used as a validation method for challenges such as determining the "true" object temperature and utilizing appropriate model parameters (e.g., physics inputs and material and simulation parameters). Levine stated that dimensional accuracy and precision can be assessed using standard test artifacts, direct dimensional measurements, round robins, standard test method development, and macroscale residual stresses measurements. He noted that macroscale residual stress measurements can also be used as validation methods while microstructure characterization and microscale residual stresses can run into unexpected problems. Also, mechanical behavior of the final part after any post-build processing could be assessed by exploring the microstructure characterization and microscale residual stresses and by utilizing mechanical testing (e.g., tensile, fatigue, and fracture).

He cautioned that many pitfalls exist with predictive simulations. Macroscale stresses can affect part shape. Local stresses can affect microstructure evolution, and local composition gradients can affect microstructure evolution. He stressed that predictive simulations need improvement in these and other areas.

Software development, integration with precision engineering, and integration into engineering workflow are also important. He stated that software can be separated into three categories:

1 High-fidelity, physics-based simulations to train computationally faster engineering simulations;
2. Pre-build engineering simulations to identify potential build problems (overhangs, thin walls, etc.) and design specific AM build process (run before each new build); and
3. Rapid, real-time, simulations for in situ adjustment of build parameters—requires feedback loop with in situ process monitoring (e.g., temperature profile, melt pool width).

He suggested that a conference series focusing on simulations for AM with computational benchmarks as a key component could benefit the community. In particular, this could be modeled after the NUMISHEET benchmarks.[1] Possible topics for discussion could include the following: single laser trace on single powder layer of known composition and size distribution (e.g., melt pool width and geometry, spatter size distribution and ejection velocity distribution, and phases present), right angle intersection of two walls (e.g., part geometry and distribution of stresses), and overhang geometry.

A DIFFERENT PERSPECTIVE ON SCALABILITY AND PUBLIC-PRIVATE PARTNERSHIP

Anthony DeCarmine, Oxford Performance Materials

Anthony DeCarmine opened by explaining that drivers to integrate computational simulation and advanced optimization methodologies to enable unique AM design exist; however, the promise of AM cannot be properly realized without the fusion of mature simulation systems and optimizers to foster migration from conventional design methodologies to a new paradigm. As it stands, few tools currently exist that enable design function to best utilize the freedoms of AM. These freedoms defeat the usual limiting assumptions of current design methods and software implementations. Current efforts from the CAD software industry reveal

[1] The website for NUMISHEET is http://www.numisheet2016.org/, accessed August 18, 2016.

acquisitions to create unions of design and analysis suites (e.g, AUTODesk with WithinLabs and ANSYS with SPACECLAIM) to achieve depth in design capabilities.

He speculated that advances in high-performance computing (HPC) capabilities for AM will likely only be brought to practical fruition by a public-private partnership because there is a lack of generally usable tools and appropriately-designed codes. He also stated that software vendors are not prepared (or perhaps willing) to migrate. A possible pathway is in software-as-service running on a shared HPC platform (such as a private cloud) or as a distributed system (e.g., SETI). He emphasized that many would-be HPC groups exist with little to no practical outcome for commonplace activity due to a lack of migration path for the developed HPC tools. Ownership of data sets, algorithms, code, and computing capacity are important considerations for partnerships. Another consideration is how (or if) to monetize the work product. He suggested that partnerships could be the home of shared services, which he described as relatively protected from market forces that drive current software business models, and could serve as licensers of developed technology.

In the general market, DeCarmine stated that there seems only to be machine makers' directives to run materials using captive or proprietary processes, which defeats the purpose of applying common or objective rules such as processing standards. This would suggest that an open or open-source approach would affect the situation positively. Unfortunately, all else being equal, the more open the AM machine system, the less likely there is to be any methodological process. He emphasized that any approach based on science would be an improvement to the general user base. An example of useful science would be the creation of a valid statistical performance basis, which provides material performance data to physically substantiate the output of HPC systems.

Discussion

Yung C. Shin, Lyle E. Levine, and Anthony DeCarmine participated in a panel discussion following their presentations, which was moderated by Slade Gardner from Lockheed Martin Space Systems Company. A national laboratory participant commented that no single U.S. entity has the expertise and financial ability to make fast and significant gains on its own; therefore, collaboration (possibly through public-private partnerships) would be helpful if the hurdles could be overcome. DeCarmine agreed that the challenge is in overcoming the hurdles. He noted that many groups in industry would be interested in contributing to a collaborative effort. Shin added that academia needs to engage in these collaborations but he worried that ownership of the outputs would pose a challenge. A participant said other models of public-private partnerships may provide some guidance, in particular the Fraunhofer Institute's system where funding is split between private sources and the German government. Another issue concerns the circumstances under which universities can participate in intellectual property relationships with industry. A participant from a national laboratory commented that there is a long history of successful public-private partnerships at NIST, and a first step would be to develop a consortium to outline key problems that need attention. Levine responded that the consortium approach is common in metal research areas, aiming to bring together industry and other researchers to solve some of the most pressing problems. An incentive put in place to participate in the consortium was to allow results generated by the consortium to be used by participating groups several years before they were available to outside groups. An academic participant referenced a collaborative effort he took part in that incentivized industry involvement by structuring one-on-one time during which industry representatives could gain individualized insights from focused academic researchers. He also noted that bringing noncompetitive industries together can prevent some conflicts.

A university participant asked about the lack of topology optimization accounting for local properties. Shin noted that topology optimization currently focuses on geometric optimization, but AM allows for materials to be tailored; therefore, materials and material properties can be optimized as well. The participant noted that some of this capability is available in existing codes.

A participant commented that a challenge of high-fidelity physics modeling is understanding and having confidence in material properties, and he wondered what NIST and other standards groups could do to help industry in this area, possibly in terms of calibration. Levine said that calibration standards are a common request across many research areas but unfortunately NIST does not have the capability to address all of these areas. He noted that suggestions are always welcome. One area of active interest at NIST is calibration standards for thermography. Developing a single reference standard is an involved process that can take 5 to 10 years, millions of dollars, and a team of experts. A participant commented that high temperature properties are an active area of interest, including developing a database of interatomic potentials. Levine responded that simulations are often not thought of as standard references but this is changing, especially with density functional theory that can quantitatively validate interatomic potentials.

A participant from a national laboratory asked for clarification on what goes into designing for AM. Shin replied that this is essentially taking advantage of the unique capabilities that AM provides to modify the design process (e.g., specifying local densities, stiffness, or thermal conductivity). These additional degrees of freedom can be used to optimize shape and performance of parts. Slade Gardner commented that Lockheed Martin has begun creating a design handbook for AM. While this has been challenging, he stated that the primary objective is to expand design for conventional manufacturing approaches.

In response to a question from the audience, DeCarmine explained that Oxford Performance Materials is a technology development company working on polymer systems. A participant commented that material supply has not been optimized for AM and few groups, with the exception of Oxford Performance Materials, are working on this area. Levine and Shin agreed, noting that using existing materials can lead to problems in AM. Levine emphasized that the economic hurdles to getting these new materials are perhaps more challenging than some of the technical constraints.

A national laboratory participant agreed that Levine's suggestion of having a benchmark for computational fluid dynamics would advance material development. Wing Kam Liu agreed and emphasized that this should be an international and collaborative effort among academia, industry, and government. Levine suggested that a first step would be to bring together a group of researchers with AM expertise to define the key challenges and identify relevant participants.

Another participant noted that topology optimization is an active research area, including multifunctional and multi-material structures, uncertainty, accuracy, feature control, overhang structure, and support design. He wondered if standards for design would be reasonable for these areas. A separate participant noted that GE has an active topology optimization program.

A participant commented that physical standards have been discussed in depth but wondered what is being done to control and manage the digital information behind physical products. Shin stated that an STL file format is typically used but agreed that more research and standardization is needed. DeCarmine noted that the ASTM F42 Committee approved a new extended file format based on a combination of STL and Extensible Markup Language (XML) that provides markup tags that can demark elements into categories (e.g., by color, texture, material). However, no machines or software manufacturers are using this new format, and some companies are developing separate file formats. He also commented that digital rights management is a challenge. A participant commented that industry groups are working on this and have partitioned the file such that only a small portion is on an individual computer at a given time.

A participant commented on public-private partnerships, noting that the vast majority of attendees at this and similar workshops are already part of some consortium on AM. These existing relationships can be used to advance many of the issues raised in this workshop.

SCALABILITY, IMPLEMENTATION, READINESS, AND TRANSITION

Rainer Hebert, University of Connecticut

Rainer Hebert explained that the powder-bed metal AM work discussed in his presentation was done in partnership with Pratt & Whitney through a joint laboratory at the University of Connecticut and in collaboration with United Technologies Aerospace Systems. He explained that the equipment included both available commercial powder-bed equipment and a new test bed (in design phase), as well as characterization equipment (including FEI Center). Also, the practical hands-on experiences were conducted as team projects with computational materials colleagues,[2] focusing on density functional theory calculations and molecular dynamics simulations.

The path for utilizing fundamental results for AM and scaling them for use in productions is complex, he explained. There are three types of fundamental results: modeling (e.g., atomic level, macro-level), theory (e.g., heat transfer, materials theory), and experiments (e.g., controlled input variables). Scaling up depends on either utilizing multiple machines of the same type or increasing build volume and throughput, both of which rely on multiple machine operators. He noted that variations in input (e.g., from machines, processes, or materials) cause variations in AM part properties (e.g., microstructures) that need to be minimized.

A key role of fundamental studies and results is to reduce variations in outcome variables while also meeting specifications, he explained. This can

[2] Colleagues include Pamir Alpay, Avinash Dongare, and other professional staff.

come in the form of fundamental studies to characterize variations in input variables or to quantify relations between input and output variables. To do this, the impact of processing and materials parameters has to be measured. Even those that do not have a measurable impact may still be useful when constructing new machines, Hebert noted. The sensitivities of important parameters (e.g., those relating to defect formation, microstructures, and machine robustness) can be used to determine the accuracy, resolution, and positions to make best use of the machines for production data.

Various combinations of theory, experiments, and simulation are needed for different areas of AM. Theoretical approaches may draw from laser theory, laser-material interactions, heat flow theory, theory of thermophysical properties, solidification (e.g., phase selection, microstructure changes, phase transformations), surface chemistry, and welding theories (e.g., spatter). Experimental approaches include laboratory experiments (e.g., laser optics such as beam characteristics and beam path control, raking) and thermophysical measurements (e.g., conductivity, specific heat, wetting angles, surface tension, viscosities, sensors, and feedback control). Applicable simulations include powder flow, Lattice-Boltzmann, density functional theory, molecular dynamics modeling, solidification modeling, and phase-field modeling.

In the short term, Hebert commented that identifying important machine, processing, and materials parameters will be a research focus. Once this is better understood, information about the microstructures and defect formation will be more easily approached. He then described six major roadblocks that hinder the scaling of AM technologies into production and use in systems:

1. Incomplete understanding of relations among materials and processing parameters, machine characteristics, and part properties and variations poses challenges. He emphasized that individual phenomena that occur during AM processes are known qualitatively but correlations and quantitative predictions for the overall process remain formidable tasks.
2. Process transparency is difficult with some machines, especially where machine parameters are opaque and hard to integrate with modeling, and beam motion settings are not known in detail.
3. Manual calibrations that some machines require create issues. While the trend is toward automated calibration and alignment routines, questions about alignment and calibration accuracies and precision will remain.

4. Machine sensing tools have limited capabilities to measure AM processes in situ as well as limited understanding of what exactly needs to be sensed and measured and at what resolution.
5. Fast machine evolutions are challenging when updates in software and hardware are not aligned with timelines for AM qualification.
6. Some drivers to promote scaling of AM technology are counterproductive for demanding applications.

There is a drive to sell and improve machines and Hebert suspects this will be accelerated when intellectual property claims expire. He stated that roadblocks 1, 4, and 6 could be addressed through additional fundamental research. This research could be partitioned into work in materials, modeling of processing aspects, experiments, and AM machines. He also noted that materials data specific to AM is needed from experiments, first-principles calculations, and simulations, including information on surface tensions, viscosities of liquid alloys, impurity effects, specific heats, thermal conductivities, and absorption coefficients. The modeling of processing aspects is also needed, including more thermodynamics and kinetics theory and Lattice-Boltzmann simulations. Macro-level heat flow theory would benefit from modeling of processing aspects such as powder raking and heat flow fluid dynamics and theory. Experiments could be used to physically simulate aspects of the AM machines and processing (e.g., raking, laser optics, powder particle melting, atmospheric effects) and improve machine control aspects, hopefully improving feedback capabilities in the future. He stated that AM machines would benefit from enhanced sensing capabilities (e.g., thermal measurements at frequencies > 1 MHz, with a heat source finder).

Hebert then discussed future applications, markets, and industry partners that may leverage the fundamental research and scale AM into production. His first example was with hybrid materials that apply different materials during one process and are often used for metal-ceramic combinations for energy applications (fuel cells), sensing applications, and coatings. Markets for these materials include energy, aerospace, and biomedical areas. He explained that fundamental research in these materials includes multicomponent diffusion, phase transformations, interface chemistries, and microstructures.

New materials specifically developed for AM applications, Hebert explained, would result in components with improved properties and could be used with high-temperature structural applications or light-weight applications, for example. These materials are particularly relevant to aerospace, automotive, and transportation markets and industries producing materials. However, fundamental research in alloy development for AM, thermodynamics, kinetics, and phase diagrams is needed.

Supporting products for AM would also benefit from additional research as industries gear up to support the transition of AM into production. From the obvious (e.g., powder) to the unsuspected (e.g., electron microscopy), the transition of AM to new applications and production levels seems to spur developments in supporting applications. Applications include measurements of AM machines and of AM-produced parts, as well as control of AM machines. Precision engineering and software markets are likely contributors with software companies offering simulation software for traditional processing and manufacturing of analysis equipment (e.g., thermal, optical, microstructure). More research is needed for the products emerging from the relevant industries that are used intrinsically for fundamental AM research.

In terms of the timeline for these research areas, he suspects that work in supporting products will continue in the short term and hopefully advance research in hybrid materials and new materials in the intermediate (5 years) and long terms (10+ years), respectively.

In conclusion, he commented that while fundamental research can be turned off instantaneously if funding is stopped, it cannot be turned on instantaneously because it takes years to build up expertise. Some of the fundamental research relevant to AM has been neglected for many years (and even decades in some cases) and it is unclear if it is still available in the United States. He also noted that a massive effort is required to stem the challenges for transitioning AM into production. The strong focus currently on the bridge from scientific research to engineering may be underestimating the real issues for transitioning AM into production.

TESTING, ACCURACY, AND BEYOND

Alonso Peralta-Duran, Honeywell International Inc.

Alonso Peralta-Duran began by explaining that he and his collaborators[3] are interested in components built with various part complexities and

[3] Collaborators include Honeywell (J. Neumann, H. Deutchman), ESI (M. Megahed), QuesTek (J. Gong, D. Snyder, G. Olson), Sigma Labs (M. Cola), and SwRI (M. Enright, J. McFarland).

functional testing substations ranging from rig to engine testing. He showed several examples of build outcomes to illustrate issues that can arise with AM, including porosity, cracking, and residual stresses, noting that capturing these behaviors in simulations is challenging. He gave an overview of the measurements of quality that are appropriate to correlate computational and analytical methods for practical implementation. The manufacturing requirements and controls are driven by and need to be commensurate with the design intent. For the most part, the requirements for components tend to be functional, dimensional (e.g., accuracy of the process, distortion due to the process, surface finish capabilities of the process), and service-life related (e.g., failure modes, material defects, material microstructure and phases, and grain size).

Computational methods must have the capability to simulate the process accurately, he emphasized. This includes replication of the process (e.g., following the laser to simulate the melting and solidification), deformation during the build to predict dimensional qualities of the process, and surface roughness. Surface roughness, he noted, is a function of the build layer thickness, the powder size distribution, the randomness of the powder spreading, the laser beam diameter, the hatch spacing, and the laser power.

Developing software architecture and databases for AM model development relies on establishing software requirements for the melt pool (e.g., modeling the power size distribution; powder spreading; laser and powder interaction; computational fluid dynamics for melting and solidification, heat transfer, and Marangoni forces; defect generation such as porosity and micro cracking; and microscale residual stresses), structure (e.g., modeling the macroscale residual stresses and deformation), microstructure (e.g., model the material microstructure evolution including phases, grain growth, and defects), and properties (e.g., yield, ultimate, fatigue, crack growth, creep, and environmental effects). Location and orientation-specific prediction capabilities also play a role. He stressed that software may be self-standing or integrated, but information must be shared.

He emphasized that more information about material properties is needed for use in computational models, including information about how materials behave from room temperature to boiling point, while in non-equilibrium conditions and under extreme operating conditions. He noted that experiments are needed to verify the relevant physics of the process, including laser scribing and melting on solid and on powder, at various processing conditions, for simple to complex shapes to determine deformation.

Peralta-Duran stressed the importance of experimental design for model validation, uncertainty quantification, and in situ process monitoring. He gave examples of some areas where this could be helpful, including laser power and size calibration, melt pool shape, pyrometer temperature measurements, build conditions, and residual stress. He also emphasized the need for software to be developed that can integrate precision engineering and engineering workflow. In particular, he highlighted two key realms of interest:

1. High-fidelity, physics-based simulations to simulate the process at the microscale and understand differences between build conditions and between geometrical differences; and
2. Computationally faster engineering simulations for component and structural simulations based on high-fidelity models.

He stressed that location-specific material properties need to be integrated into current finite element codes and analysis and that manufacturing groups need to be engaged in future developments.

COMPUTATIONAL SIMULATION AND ADVANCED OPTIMIZATION: THE KEY ROLE OF PUBLIC-PRIVATE PARTNERSHIPS IN SCALABILITY

Tahany El-Wardany, United Technologies Research Center

Tahany El-Wardany began with an overview of United Technologies Research Center (UTRC) where she and her collaborators[4] partner with other business units within United Technologies, including Pratt & Whitney, Sikorsky, UTC Building and Industrial Systems (Otis and UTC Climate, Controls, and Security), and UTC Aerospace Systems. Each of these business units is focused on separate technologies, which incentivizes the use of multiple AM approaches (e.g., AM with cold spray, wire arc, laser powder-bed fusion, laser powder deposition fusion, and electron beam melting). UTRC aims to define new frontiers, codevelop technologies, solve tough problems, serve as a hub for technical interchange, leverage a global network of innovation, and monetize UTC intellectual property. She explained that UTRC develops multiphysics, multiscale models for

[4] Collaborators include Ranadip Acharya, Sergey Mironets, Matthew Lynch, Vijay Jagdale, Ken Smith, G.V. Srinivasan, Alex Staroselsky, John Sharon, and Bill Tredway.

advanced manufacturing technologies with the goal of improving product quality, performance, and cost.

She discussed drivers to integrate computational simulation and active operations management. Three major challenges in the AM process include distortion, origination of defects and microstructure and their effect on fatigue, and defects. She posed two considerations:

1. At what point are material properties more influenced by defects than by the microstructure (e.g., grain size and orientation, anisotrophy)?
2. To what extent does the initial microstructure from AM processing impact the properties of the final post-processed component?

Leveraging and integrating tools to get the best possible product is a challenge. The goal is to predict the right process parameters of the first part while optimizing process parameters, geometrical accuracy, mechanical and metallurgy properties, building time, and cost. However, El-Wardany described some near- and long-term development and integration efforts that are still needed, including the following:

- Material models
  - *Near term*: powder characteristics and representation
  - *Longer term*: physical properties, thermal mechanical behavior, metallurgy and rheology, and layout of functional grading in materials
- Design
  - *Near term*: part geometry, support structure
  - *Longer term*: no support structure
- Process physics
  - *Near term*: multiphysics simulation of AM process, energy source representation and interaction parameters
  - *Longer term*: possible onset and propagation of defects, part specific control of defects, interfacial characteristics
- Processing of geometric model
  - *Near term*: slicing and path generation, optimizing process through designed experiments
  - *Longer term*: tailoring of process characteristics for desired properties

- Equipment environment as model input
  - —*Near term*: machine motion and scan parameters, chamber process atmosphere
  - —*Longer term*: shape and characteristic angle of deposit, in-process monitoring, and closed-loop feed back

Several needs for advancing simulations are interconnected, such as designing a part for the AM manufacturing process, engineering materials for the design, and specifying and optimizing process parameters for material properties and design. Computational tools include part design and analysis (e.g., finite element analysis, computational fluid dynamics, level set, and multiphysics analysis), manufacturing characteristics (e.g., CAD and morphing), and material properties (e.g., multiscale simulations). She explained that optimization is also often done by linking codes and simultaneously considering design, manufacturing, and materials.

HPC modeling and simulation capabilities are essential for AM large-scale modeling, El-Wardany explained. She suggested that standards for HPC collaborations among universities, national laboratories, and industry are needed to advance the AM large-scale modeling of microstructure and material properties.

Also, she explained that opportunities exist for public-private partnerships to advance HPC capabilities, enhance the ability to add different constraints during the design stage of AM parts, and augment the computation of different multiscale phenomena and enable smoother coupling between them for large scale modeling that predicts material properties and mechanical behavior. Partnerships could also help facilitate the development and execution of high-fidelity models of complex features such as microstructure evolution during rapid solidification in AM, she stated. Integrated computational material engineering (ICME) and large data managements would also benefit from partnerships, as would technology transfer through the supply chain and into the aftermarket.

These partnerships stand to benefit from AM advancements, El-Wardany noted, especially with respect to developing the mechanistic understanding of materials behavior during layered manufacturing to enable unique design optimization, generating new commercial off-the-shelf tools that can be applied for microstructure and mechanical property prediction, developing preliminary design curves for new materials with minimum experimental cost, and linking materials and process models to support probabilistic design capabilities.

Future processing standards are also a consideration, she explained. She said that processing standards often change with each analytical and mechanistic model approach. The standards need to reflect the mechanical property models developed to support materials, processing properties relationships, and AM component design. The inclusion of a physics-based model in the process framework may improve the chance of the first part being produced correctly. She noted that real-time feedback control of the process model is required.

In conclusion, she emphasized that the evolving AM paradigm requires ICME and optimization with physics-based models and topology optimization. Concurrent hybrid processes can be implemented to include process monitoring, online inspection, feedback control, and virtual manufacturing workflow optimization.

Discussion

Following their presentations, Rainer Hebert, Alonso Peralta-Duran, and Tahany El-Wardany participated in a joint panel discussion moderated by Anthony DeCarmine, Oxford Performance Materials. The first question came from a national laboratory participant who asked about the impact of large powder particles. Peralta-Duran responded that large particles impact the surface roughness for two reasons: the spreading of the large particles disrupts the melt pool dynamics, and the large particles may not melt entirely and therefore protrude from the surface.

A participant asked about the panelists' experiences using multiple machines. Hebert responded that he and his collaborators use several different machines and have noticed differences in the robustness of the machines. It is difficult to do direct machine comparisons because they use dedicated powder intended for each machine.

A participant asked about taking manufacturing into consideration when doing topology optimization. El-Wardany responded that this is particularly important for some AM approaches, such as is the case with cold spray and its fixed spray angles. The parameters that need to be designed for include structural supports, surface finish, and available power. Another participant noted that reference material on design rules for AM processes would be helpful to guide researchers in these areas.

An online participant noted that many of the computational approaches discussed in the workshop have had long run times and wondered what faster simulation approaches show promise. A previous speaker commented that differences between the faster and slower computations come down to explicit and implicit time integration. Much of the commercial code simulations are slower because the typical thermal problem requires implicit time integration to resolve the time scale of the phase change. Peralta-Duran commented that this is not always the case and modeling assumptions and decisions are often employed to simplify and therefore speed the computation. While this can limit predictive capabilities in some cases, he explained that these simplified simulations can be used to model many types of behaviors effectively. El-Wardany added that there is also the potential to expand these codes to solve a variety of problems, including physics problems.

A participant asked El-Wardany to elaborate on near-term material models for material characteristics being developed at UTRC. She explained that they developed procedures for powder and wire deposition characterization. They do not have models for powder deposition but they are using experimental data that can closely represent the powder behavior.

Another participant asked how to separate the base plate from the build and whether this induces stress or distortion. Peralta-Duran commented that Honeywell has been using wire-cut electrical discharge machining, which does not seem to induce notable stress or distortion.

An online participant asked about priorities for the process parameters. El-Wardany said the power velocity ratio (or power density function of the velocity) is usually the first parameter UTRC considers because it impacts the geometry. They then typically look at the hatch spacing. However, she noted that there are over one hundred variables and at least a quarter of them have to be accounted for in a model. Peralta-Duran added that the priorities depend on the model objectives.

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Summary of Issues from Subgroup Discussions

During the third day of the workshop, participants met in subgroups to discuss some of the challenges and possible solutions to the questions set forth for each session. Summaries of the subgroup discussions are provided in the following subsections.

THEORETICAL UNDERSTANDING OF MATERIALS SCIENCE AND MECHANICS

Subgroup Members

Steve Daniewicz (Mississippi State University), Marianne Francois (Los Alamos National Laboratory), Edward H. Glaessgen (NASA), Neil Hodge (Lawrence Livermore National Laboratory), Saad Khairallah (Lawrence Livermore National Laboratory), Peter Olmsted (Georgetown University), and John Turner (Oak Ridge National Laboratory).

Summary

Several members of the subgroup mentioned the importance of developing a scientific methodology integrating theory, modeling and simulation, and experiments toward prediction and control, which could benefit the broader additive manufacturing (AM) community. They discussed fundamental scientific issues of AM to be addressed in the future and identified a number of topics for more research, including the following:

- Strongly non-equilibrium processes (e.g., high rates of flow, energy deposition rates, phase transformations),
- Mechanics of strongly heterogeneous materials (e.g., varying porosity, microstructure and orientation, composition),
- Multiple simultaneous processes (e.g., heat, fluid, particle flow, phase changes, stress-strain including crystal plasticity), and
- Experimental material design utilizing information science.

Subgroup members also made several observations about the state of fundamental science in AM. Some stated that the qualification cycle could be shortened by utilizing a scientific-based approach, while others noted that computational thermodynamics as a field needs more depth and breadth.

Microstructure variation was highlighted by many subgroup members as a major challenge. They commented that AM processes produce different microstructures from traditional manufacturing processes. There seems to be two length scales: the weld beads and the length scale of individual grains (smaller than the weld bead). The difference in microstructure (e.g., orientation, crystal phase) results in very different properties and damage processes. They also noted that certification is challenging given that durability and life cycle performance result from microstructural variability, residual stress, and defects.

Several opportunities for utilizing multiple materials with AM were discussed during the workshop. Several members of this subgroup noted that current methods, expertise, and machines are typically focused on a single material or class of material. In the future (10+ years) they hope that these approaches will be linked together to develop hybrid materials (e.g., organic/inorganic materials, multiple materials, aqueous and biological materials). One challenge to achieving this is minimizing abrupt interfaces between dissimilar materials. They suggested that simulations could be developed to account for and enable optimization of such gradient interfaces. They also commented that multiple metastable crystalline states arise from many-component alloys under strong non-equilibrium conditions.

The subgroup also discussed the mathematical models and state-of-the-art theoretical, computational simulation models that describe the different aspects of AM that exist or are needed to simulate the various stages of AM. The group began with a discussion of microstructure-aware continuum dynamics code, both for material processing (e.g., modeling and simulation of solidification) and performance modeling (e.g., thermo-mechanical, elasto-plastic). A number of participants emphasized the need to develop new methods in phase field modeling to capture the microstructure in the non-equilibrium and dynamical environment prevalent during an AM process. Starting with some challenges, they highlighted that high-performance computing does not work well with the numerical methods for the stiffness matrix calculations. Others noted that many multiphysics (e.g., heat transfer, fluid flow, solid mechanics) and finite element structural analysis codes already exist but more efficient, accurate, and robust numerical methods with implicit solvers would be useful, as would additional reduced-order models and computational techniques for multiscale methods. They also emphasized that models are needed for melt pool dynamics (e.g., interface tracking method with phase change), as are phase-field models for microstructure evolution. Lastly, some of the subgroup noted that data-based analysis could to help elucidate trends and possibly provide process bounds for AM users.

Another topic discussed was the integration frameworks that currently exist for coupling modeling techniques together. Some subgroup members noted that the Materials Genome Initiative (MGI)[1] offers a paradigm that fits well with the needs of AM. MGI is built around identifying how specific materials lead to different end properties, via different processes. It links multiple scales, from quantum and atomistic to molecular mechanics and derived potentials, to mesoscale (nanometer) methods, and finally to continuum level. Process characteristics and effects play an integral role in the genome of a material. A similar approach to unite scales and methods is appropriate for AM, these individuals emphasized. With AM, the microstructure of the material could be tailored to specific requirements and needs, which provides for many opportunities of material design.

Many members noted that there are no software suites that contain all of the functionalities necessary to model all aspect of various AM processes. Even existing tools often do not consolidate well with each other.

Recent multi-institutional programs have demonstrated that collaborative development of simulation environments aimed at solving complex problems can successfully deliver capabilities that would otherwise not be possible, several participants explained. Examples include the following:

[1] The website for the Materials Genome Initiative is http://www.mgi.gov, accessed August 23, 2016.

- The Consortium for Advanced Simulation of Light Water Reactors (CASL),[2] which serves as the Department of Energy (DOE) Innovation Hub on modeling and simulation for nuclear energy;
- DOE's Accelerated Climate Modeling for Energy (ACME) program;[3] and
- DOE/EM Advanced Simulation Capability for Environmental Management (ASCEM).[4]

A number of subgroup members observed that a similarly coordinated effort for AM could benefit the development of common input and output formats, thereby reducing necessary end-user effort to perform analyses. It could also aid the development of common interfaces for physics components, which could facilitate the sharing of models. These individuals noted that such an effort would also leverage existing simulation tools, enable researchers to focus on their areas of expertise without having to create other required components, and provide the ability to explore coupled and multiscale interactions. Ideally, they said, such environments could also provide both reduced-order and high-fidelity models and implementations able to run on systems ranging from workstations to the largest HPC platforms.

Several subgroup members identified what they viewed as the most important open questions in materials and mechanics, including related scientific disciplines, engineering and mathematics, as well as the technical challenges to be addressed for predictive theoretical and computational approaches in order to enable widespread adoption of AM. In doing so, they listed some areas of fundamental research in theoretical and computational materials science, mechanics, and multiscale computation that could advance AM:

- *Polymer FDM (P-FDM).* Fundamental polymer science issues include the glass transition, the flow-induced crystallization, and the relationship between complex microstructure and mechanical properties.

[2] The website for the Consortium for Advanced Simulation of Light-Water Reactors is http://www.casl.gov/, accessed August 23, 2016.

[3] The website for Accelerated Climate Modeling for Energy is http://climatemodeling.science.energy.gov/, accessed August 23, 2016.

[4] The website for Advanced Simulation Capability for Environmental Management is http://esd1.lbl.gov/research/projects/ascem/, accessed August 23, 2016.

- *Build region/melt pool level.* Fundamental issues include orientation prediction, glassy and semi-crystalline morphology as appropriate, and resulting strength, weld properties, local moduli, and heat transfer and processing conditions (e.g., speeds, flow rates, temperature, geometry).
- *Part level.* Key challenges relate to predicting, designing, and controlling the overall mechanical and structural properties. Some members noted that it would be extremely helpful if part-scale models could run in two different modes: (1) high-resolution, suitable for detailed determination of the solids response, and (2) fast, which would be able to execute much more quickly, at the cost of solution accuracy. Once mode (2) is realized, it would be useful to link the simulations to process-informed topology and function optimization, which would also need to be able to handle material and geometric nonlinearities (which they currently cannot do) to be really useful.
- *Metals.* High-fidelity physics-based models face challenges with their processing, properties, and performance. Processing improvements would help to model melt pool dynamics, melting and solidification cycles, mass and energy deposition model, and alloy composition distribution for multiple components. It would also be beneficial to include G&R map in solidification modeling as well as model microstructure-aware solidification. These models cannot yet predict strength properties of AM metals (as discussed by Bishop and Francois), but several subgroup members stated that their development would be helpful. Performance challenges mentioned related to plasticity, damage, and durability models.
- *Linkage.* Linking scales and models is also a challenge, including connecting phase change models through thermodynamic calculations and linking microstructure information to macroscale models.
- *Materials.* Some subgroup participants emphasized that the future of AM eventually might be dominated by material questions because there are limitless ways of combining materials. Potential issues include (1) determining optimal powder materials and alloys to use for a given application, (2) understanding how physical properties change (e.g., hardness, strength) when different materials melt and solidify under AM-prevalent non-steady-state conditions, and (3) printing functional products that consist of printed or embedded electronic components or functional organics for biological application.

- *Mathematics.* Several relevant mathematical issues were discussed, including statistical methods, machine learning algorithms, pattern recognition, database and data science, applied mathematics (e.g., coupling of partial differential equations, time integration schemes, higher-order discretization methods, implicit solvers), and multi-scale methods (e.g., coarse graining, discrete-continuum).

Multidisciplinary and related materials and mechanical sciences needed for AM were also discussed, including computational modeling, metallurgy, mechanical and chemical engineering, physics, chemistry, data analytics, and computer science. A number of subgroup members stated that the field will benefit from large teams working together to link different length and time scales, as well as different arenas of interest (e.g., material, deposition methodologies, metrologies, modeling, testing and validation, design).

Regarding verifying and validating theoretical and computational models for AM processes, many subgroup members noted that computational and AM-build benchmarks are needed and that AM-build benchmarks would be of great interest to standards organizations to address variability within AM processes. In the short run, they noted that validation of simulations could be done via classical methods such as creating and characterizing parts against model results. Ostensibly, they said this should start with fairly simple geometries and proceed to increasingly complex problems. In the context of the small scale, this could consist of single-track experiments. At the part scale, it could start with small parts (e.g., 1 mm^3), and increase to a medium-sized part with a few features (e.g., cm^3, with some holes, overhangs, and interior passages), and then finally to a large, complex part (e.g., 4-cylinder engine block).

Several group members also noted that in situ monitoring and diagnostics could be improved through increased access to real-time data, with data analytics, or by state-of-the-art characterization. This might include exploiting big data techniques to deepen the validation process, such as using reconstructed images and or diffraction data. They noted that there is a strong need for on-line in situ metrologies to be built in as standard on equipment (e.g., temperatures, molecular and microstructural information, microscopies). In the long term, they hoped to see in situ metrologies linked to high-performance computing and modeling to adjust and optimize the design and build on the fly in real time. These members also emphasized that the development of standard benchmark cases (simple to complex) to test computational methods and code would be helpful, as would open-source and published computational algorithms and physics models. An example for simple test cases could be a single-track pass for a powder-bed machine and a LENS system, where the metrics of interest (e.g., temperature history and melt pool shape) are developed and can be used for comparison. Such comparison exercises would drive improved quality of computational methods and software.

A number of subgroup members suggested possible opportunities for public-private partnerships to advance theoretical and computational mechanics capabilities for AM, the first of which being internships and doctoral student networks to provide interdisciplinary training. They also noted that it is important to link materials producers (e.g., powders, FDM filaments, and grains), equipment manufacturers, metrologists, computational and theoretical modelers, end users and developers, and standards bodies to increase communication and collaboration while accommodating the groups' various interests. In particular, they suggested potential focuses of partnerships, such as developing physics models and numerical methods, implementing models and methods in software, and performing validation. One concern these participants raised was whether creative partnerships could be developed to preserve individual intellectual property. They emphasized for the value of specific public-private partnership calls that span government organizations (e.g., National Science Foundation [NSF], Department of Energy [DOE], Department of Defense [DoD], and National Institute of Standards and Technology [NIST]), commenting that DOE's newly-announced High-Performance Computing for Manufacturing (HPC4Mfg) program[5] provides a possible model for industry-driven collaboration on shorter-term needs. A complementary longer-horizon program focused on R&D challenges in materials science, applied mathematics, and numerics, and on development of a community simulation environment would accelerate progress further, they observed, ideally influenced by lessons learned in HPC4Mfg.

Several subgroup members noted that partnerships would benefit from the strengths of the other groups and the fundamental scientific and engineering baseline would be raised so that all partners would be able to operate more efficiently and more flexibly. Academic researchers would bring expertise and advanced training opportunities to the partnerships, for example. National laboratory partners could provide high-performance computing capabilities

[5] The website for High-Performance Computing for Manufacturing is https://hpc4mfg.llnl.gov/, accessed August 23, 2016.

and user experimental facilities. Industry partners could gain insight from their product experience and also provide funding opportunities.

Many group members emphasized the variability in processes and materials and the need for standards in measurement, process, and materials. The development of sophisticated predictive modeling that relies on sound metrology and materials could in turn lead to a positive feedback that would encourage new standards. They explained that theorists and modelers need a full understanding of life cycle process and well-characterized model materials. A push to understand properties based on these details could lead to a better understanding of how to design functionality more rapidly and efficiently. These members also stressed the importance of coordination and acceptance from certification authorities (e.g., the Federal Aviation Administration [FAA]).

In terms of policy, some subgroup members noted that visible and prominent challenges have the potential to capture the public's imagination, analogous to the XPRIZE[6] where a large monetary prize could focus the imagination and attract large investment. They commented that AM can be linked to societal needs such as energy, climate, personalized medicine, and sustainability, with potential for a wider engagement.

Future needs for AM were also discussed by the subgroup. Given the high speeds (especially of selective laser melting processes), feedback control may not be fast enough to make process corrections in real time, several observed. One possible way to improve in situ corrections would be to use small, idealized simulations to predict process and estimate process parameters ahead of time.

Computational and AM-build benchmark tests were also discussed. Specifically, some subgroup participants mentioned the need for a common test bed with multiple challenge problems to build confidence in simulations and AM builds, observing that AM-build benchmarks would be of great interest to the ASTM F42 Committee on Additive Manufacturing. They envisioned two classes of test problems:

1. *Benchmark problems.* These would be well-defined problems, ideally a progression from simple geometries with single materials with well-known properties designed to test a single physical phenomenon up to complex geometries, including diverse materials, multiple scales, and physical phenomena. Details of initial and boundary

[6] The website for XPRIZE is www.xprize.org, accessed August 23, 2016.

conditions, along with characterization data, would be available to the community. These data would provide common verification and validation information against which models could be compared, enabling trade-offs between fidelity and computational resource requirements. The benchmark problems might also drive development of new experimental techniques to provide data that is currently unavailable. Data and results could be provided through a DOE national laboratory or other institution.

2. *Challenge problems.* These would typically be driven by real-world needs and might not be possible currently, either physically or virtually. They might include extremely complex geometries, materials that may not exist, and multiple physical phenomena, these participants said. Some of these problems might be similar to the XPRIZE concept mentioned above and would serve to both inspire and drive R&D activities. A few subgroup members noted that standards organizations such as ASTM E08 and F42 work commonly with coupons, but simulations are needed to bridge the gap between coupons and components.

Several subgroup members commented that workshop presentations repeatedly mentioned the various parameters describing melt pool solidification rate or heat input, which can be used to describe a successful build. They wondered if computational simulations could be used to define a nondimensional parameter that is more powerful than the currently known parameters.

COMPUTATIONAL AND ANALYTICAL METHODS IN ADDITIVE MANUFACTURING

Subgroup Members

Corbett Battaile (Sandia National Laboratories), Joe Bishop (Sandia National Laboratories), Wayne King (Lawrence Livermore National Laboratory), Anthony Rollett (Carnegie Mellon University), David Snyder (QuesTek Innovations), and Gregory Wagner (Northwestern University).

Summary

Several of the subgroup members discussed unique characteristics of AM including the capability for material design, specifically with respect to alloy design. However, they noted a number of challenges including difficulties with CAD and surface representation that often rely on nonparameteric surfaces, point clouds, and implicit surfaces where tolerances can only be applied at interfaces. Concerns about corrosion and surface effects can also cause issues for AM build, tribology, and wear. Some subgroup participants noted that AM has several unique design constraints, such as overhangs and a top-down identification of processing. They described the lack of fundamental understanding of process, structure, and material properties, design of alloys specific to AM (accounting for non-equilibrium thermodynamics from high cooling rates), physics-based process control (both feed-forward and feed-back), and accounting for surface effects at all scales (chemistry and interfacial chemistry, surface finish). Some of the technical concerns include determining what combination of powders will result in desired material properties, how to control material grading (e.g., temperature gradients), and what relationships would scale across machines, alloys, laser heat inputs, and different beam sizes and energy density. These individuals stated that process control and length scale effects (e.g., exotic microstructures, high-temperature measurements, high-cooling rates, unique processing) and powder and laser interactions are not being well studied.

To move beyond these issues and advance the use of AM, members of the subgroup discussed the importance of designing parts that minimize residual stresses and snap back by design. Many participants stressed the value of integrating multidisciplinary optimization into a build, including topology, shape, material, manufacturing, uncertainty quantification, residual stress, build path, and feedback. They noted that advanced macroscale viscoplastic material models are also needed. These participants also stated that computational material science could be used to reveal mechanisms and for process design. Physics-based process control, whether feed-forward or feed-back (enables robust AM independent of machine), could allow for advances in microstructure-based process control and residual stress control.

They also commented on the importance of multidisciplinary optimization such as how to integrate different tools sequentially, considering topology, shape, material, manufacturing, uncertainty quantification, residual stress, and AM build path. These participants highlighted the merits of multiscale modeling (e.g., computational homogenization), predictive crystal-plasticity, and material thermodynamics for novel AM microstructures. Also, improved estimation and control of modeling errors on engineering quantities of interest (e.g., from material models) would be helpful, they explained.

Some subgroup members noted that many of the fundamental science questions reside in applied research areas, such as better understanding the melt pool physics and powder interactions. They also commented that HPC is transforming physics-based codes to take advantage of new architectures. Areas for opportunities include better use of big data, data compression (e.g., optimal representation, basis), and surrogate models.

Modeling and simulation for advanced and complex production would be helpful, members of the subgroup stated. Creating and using a fully predictive model is often too expensive but statistical methods could be used to gain more insight. Surrogate and reduced models derived from HPC models show promise for industrial use, especially those that focus on residual stress, prediction, control, and minimization. New models and software might have value, including advanced macroscale viscoplastic models with internal state variables capable of modeling processing history and new CAD representations for AM. These individuals also emphasized the benefits of HPC and exascale computing in support of uncertainty quantification and error estimation, Bayesian methods, optimal experimental design, data fusion in real time, and improved control of machine-to-machine variability. They commented on the importance of accelerating advanced software for industrial use.

Subgroup members also discussed the lengthy time currently required for part qualification. They believe that focusing on high-sensitivity parameters as well as utilizing advanced diagnostics and the processing history of each point in build (where statistics of each point over ensemble of builds can be used) could accelerate this process. These advances could help qualify each part by understanding the precise processing history of each point, while also improving first-run builds, these members explained.

Other subgroup members said that a science-based theory of AM capabilities could help researchers observe characteristics that are difficult to measure. They noted that data science for AM material systems discovery has potential, including data mining, discovery of emergent behavior, mechanistic-based data compression, high-throughput standardization, and quantitative material testing. The benefit of establishing an AM database for both experimental and modeling and simulation, similar to MGI, was also discussed by these participants. They noted that the community could benefit from more openly available data and software for enhanced use in data informatics and material models.

Many of the subgroup members emphasized the importance of developing interdisciplinary degree programs and fellowships for AM.

They stressed that AM processes rely on different design rules and require different ways of formulating problems. Lastly, they stated that it is challenging but important to bridge the gap between fundamental science and manufacturing.

MONITORING AND ADVANCED DIAGNOSTICS TO ENABLE AM FUNDAMENTAL UNDERSTANDING

Subgroup Members

Joseph Beaman (University of Texas at Austin), Jian Cao (Northwestern University), Feng Lin (Tsinghua University), Ade Makinde (GE Global Research Center), Z.J. Pei (National Science Foundation), Edwin Schwalbach (Air Force Research Laboratory), and Yu-Ping Yang (EWI).

Summary

Many subgroup participants began by emphasizing the importance of modeling and sensing for prediction and operation. However, they noted that several challenges were not discussed during the workshop, including the importance of the measurement matrix for different simulation tools and the fact that the closed nature of the machines makes it difficult to access the complete data history of machines. They also mentioned the challenges of testing and examining internal features of AM parts, such as identifying the voids in thin walls particularly when the tolerable pore size is just one order smaller than the feature size.

Several members of the subgroup offered short-, mid-, and long-term goals. In the short term, which they defined as up to the next two years, goals could be to (1) identify the correlation between defects and signals of interest, including developing algorithms for combining in situ sensing with post-built measurement and theory for signal processing and data mining; (2) understand and characterize thermodynamic behavior of metals and surface tension through thermal-mechanical modeling (high temp properties, high thermal gradient) and microstructure modeling; (3) develop national facilities with open-architecture and highly-instrumented machines; (4) study the fundamentals of AM processes with the help of advanced metrology such as in situ X-ray and neutron measurement and the development and integration of low-cost sensors for gas current measurement; (5) improve sensing for health monitoring of machines; (6) improve temperature measurement accuracy (within 50°C) over the entire bed; and (7) improve simulation tools for powder spreading.

Mid-term goals (in the next two to five years) discussed by these subgroup members were to (1) further improve temperature measurements (within 10°C) over the area; (2) better integrate modeling with different sensing modalities (e.g., laser interferometer, inferred, pyrometer, microstructure, ultrasonic for porosity, X-ray) with statistical methods; (3) develop algorithms for integrating the sensing needs and capabilities into the design of the part; (4) further develop model-based reconstruction techniques for CT scan; (5) improve simulation tools for powder development; and (6) explore methods for defining function-driven metrology needs.

Long-term goals for the next five to ten years discussed by these individuals were to (1) develop a fully-coupled model; (2) improve in situ identification of gradient material structure, and (3) develop a digital thread for each part (e.g., data analytics, materials, process, and performance and failure in the field and application).

These subgroup members suggested that fundamental research to drive next-generation AM processes be a consideration as well as optimization of AM parts with functionally-gradient materials (e.g., local material design, topology design, re-separate and recycling of powders). Lastly, they emphasized the value of graduate fellowships and industrial summer internships for advanced AM. They stressed that the continuation of fundamental research for AM would continue to move the field forward.

SCALABILITY, IMPLEMENTATION, READINESS, AND TRANSITION

Subgroup Members

Anthony DeCarmine (Oxford Performance Materials), Tahany El-Wardany (United Technologies Research Center), Rainer Hebert (University of Connecticut), Lyle E. Levine (National Institute of Standards and Technology), Alonso Peralta-Duran (Honeywell International Inc.), and Yung C. Shin (Purdue University).

Summary

The subgroup members began with a discussion of the path for utilizing fundamental results for AM and scaling them for use in production.

Some members of the subgroup suggested that the accurate representation of feedstock, energy, environment, and kinematics of machines is important and could be accounted for, and the impact of energy inputs (e.g., laser beam profile, time-power behavior) and interactions of beams with materials could be better understood. The effect of the parameters on the interaction with materials and the resultant microstructure and phases, and the difference in melting and flow behavior between spherical and non-spherical (or satellite) particles, could also be better understood.

The main roadblocks some of these participants see in the scaling of AM technologies into production is the lack of hierarchical high-fidelity models, including hierarchical engineering models. They commented that too much time is often spent on one length scale without relation to higher level length scales. High-fidelity, physics-based simulations could be used to train surrogate reduced-order models. Also, pre-build engineering simulations could be run before each new build and the results could be used to identify and correct potential build problems. They noted that rapid simulations for in situ fine tuning of build parameters require a feedback loop with in situ process monitoring (e.g., temperature profile, melt pool width), possibly after each layer is deposited.

In terms of addressing these roadblocks through additional fundamental research, members of the subgroup stated that high-fidelity models could be developed for various AM processes as could reduced-order models that are more computationally efficient. They also emphasized that the establishment of mechanisms for longer-term collaborative efforts among researchers in academia, government, and industry would be helpful, as would the establishment of a repository or database for material selection, properties, or response surfaces. These subgroup members also suggested the development of a software test bed for benchmarking different AM software.

To leverage the fundamental research and scale it into production, other subgroup members suggested that the software companies become involved in developing open architecture and partnering topology optimization with AM machine design. Research would be valuable to better address support structures and design of geometrical features for use in ceramic applications and coatings.

Measurements of quality or systems that correlate computational and analytical methods to practical implementations were also discussed by several subgroup members. These members identfied geometry, microstructure, defects, mechanical behavior, environmental behavior (corrosion), part qualification, standards, and machine qualification or standards as aspects that would benefit from more input.

Software architecture and databases for AM model development were mentioned by subgroup participants. They suggested leveraging the existing efforts in the MGI for AM to develop databases of software and parameter data. They also noted that MGI works in a design space that is a subset of the design space where AM operates, but AM adds high heating and cooling rates. These participants suggested using scalable software with a hierarchical (modular) approach and a hierarchy of engineering simulations. Benchmark test series, they noted, could pull independent research groups together and identify effective modeling, measurement, and AM strategies.

Other subgroup members noted that careful design of validation experiments for model validation, uncertainty quantification, and in situ process monitoring is challenging because there is a lack of data for probabilistic modeling and error estimation. Test standards and test artifacts would help, as would an adequate suite of in situ monitoring to provide useful engineering data, they explained.

These subgroup members emphasized that there are drivers to integrate computational simulation and advanced optimization methodologies to enable unique AM design, and full life cycle simulations are important for qualifying AM-built parts. They noted that processing standards might change with an analytical and mechanistic model approach to implementation of full-scale AM.

Several other subgroup members described opportunities for public-private partnerships to advance HPC and other capabilities for AM. These partnerships are important to define and implement hierarchical models that are developed based on exchanges among industry, national laboratories, and universities. They emphasized that the proposed benchmark test series may present a mechanism for a public-private partnership. Partners could benefit from advancements within partnerships by having access to focused research with shared guidelines. Industry could focus on practical AM while national laboratories and academia could provide feedback on what to focus on and provide expertise on what can or cannot be measured experimentally.

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Appendixes

Appendix A

Registered Workshop Participants

Corbett Battaile, Sandia National Laboratories
Joseph Beaman, University of Texas at Austin
Joe Bishop, Sandia National Laboratories
Jian Cao, Northwestern University
Gengdong Cheng, Dalian University of Technology
Steve Daniewicz, Mississippi State University
Anthony DeCarmine, Oxford Performance Materials
Edward Dobner, Deloitte Consulting
Tahany El-Wardany, United Technologies Research Center
Marianne Francois, Los Alamos National Laboratory
Edward Garboczi, National Institute of Standards and Technology
Slade Gardner, Lockheed Martin Space Systems Company
Edward Glaessgen, National Aeronautics and Space Administration
Langley Research Center
Xu Guo, Dalian University of Technology
Rainer Hebert, University of Connecticut
Martin Heinstein, Sandia National Laboratories
Neil Hodge, Lawrence Livermore National Laboratory
Linda Horton, United States Department of Energy Office of Science
David M. Keicher, Sandia National Laboratories
Saad Khairallah, Lawrence Livermore National Laboratory
Wayne King, Lawrence Livermore National Laboratory
Lyle E. Levine, National Institute of Standards and Technology

Feng Lin, Tsinghua University
Wing Kam Liu, Northwestern University
Li Ma, National Institute of Standards and Technology
Ade Makinde, GE Global Research Center
Kalman Migler, National Institute of Standards and Technology
Peter Olmsted, Georgetown University
Tim Osswald, University of Wisconsin–Madison
Zhijian Pei, Kansas State University
Alonso Peralta-Duran, Honeywell International Inc.
Kara Peters, North Carolina State University
Michael Plesniak, The George Washington University
Richard Ricker, National Institute of Standards and Technology
Anthony Rollett, Carnegie Mellon University
Edwin Schwalbach, Air Force Research Laboratory
Yung C. Shin, Purdue University
John Siemon, Alcoa Technical Center
Ole Sigmund, Technical University of Denmark
David Snyder, QuesTek Innovations
David Stepp, United States Army Research Laboratory
Amy Sun, Lockheed Martin Space Systems Company
Stuart Trouton, Deloitte Consulting
John Turner, Oak Ridge National Laboratory
Max Voegler, Deutsche Forschungsgemeinschaft
Gregory Wagner, Northwestern University
Ian Wing, Deloitte Consulting
Kristopher Wise, National Aeronautics and Space Administration Langley Research Center
Peter Wriggers, Leibniz Universität
Yu-Ping Yang, EWI

Appendix B

Workshop Agenda

DAY 1: OCTOBER 7, 2015

8:00 a.m. **Introduction**
Wing Kam Liu, Northwestern University (Chair of the U.S. National Committee on Theoretical and Applied Mechanics and chair of workshop planning committee)

8:15 a.m. **Session 1: Theoretical Understanding of Materials Science and Mechanics**
Facilitator: Wing Kam Liu, Northwestern University
Speakers: Marianne Francois, Los Alamos National Laboratory
Peter Olmsted, Georgetown University
John Turner, Oak Ridge National Laboratory

10:15 a.m. **Session 2: Computational and Analytical Methods in Additive Manufacturing**
Facilitator: Steve Daniewicz, Mississippi State University
Speakers: Anthony Rollett, Carnegie Mellon University
Wayne King, Livermore National Laboratory
Corbett Battaile, Sandia National Laboratories

1:15 p.m. **Session 3: Monitoring and Advanced Diagnostics to Enable Additive Manufacturing Fundamental Understanding**
Facilitator: Anthony DeCarmine, Oxford Performance Materials
Speakers: Ade Makinde, GE Global Research Center
Joseph Beaman, University of Texas at Austin
Jian Cao, Northwestern University

3:30 p.m. **Session 4: Additive Manufacturing Scalability, Implementation, Readiness, and Transition**
Facilitator: Slade Gardner, Lockheed Martin Space Systems Company
Speakers: Yung C. Shin, Purdue University
Lyle E. Levine, National Institute of Standards and Technology
Anthony DeCarmine, Oxford Performance Materials

5:15 p.m. **Adjourn Day 1**

DAY 2: OCTOBER 8, 2015

8:15 a.m. **Session 5: Theoretical Understanding of Materials Science and Mechanics**
Facilitator: Wing Kam Liu, Northwestern University
Speakers: Steve Daniewicz, Mississippi State University
Neil Hodge, Lawrence Livermore National Laboratory
Saad Khairallah, Lawrence Livermore National Laboratory

10:15 a.m. **Session 6: Computational and Analytical Methods in Additive Manufacturing**
Facilitator: Steve Daniewicz, Mississippi State University
Speakers: David Snyder, QuesTek Innovations
Gregory Wagner, Northwestern University
Joe Bishop, Sandia National Laboratories

1:15 p.m. **Session 7: Monitoring and Advanced Diagnostics to Enable Additive Manufacturing Fundamental Understanding**
Facilitator: Slade Gardner, Lockheed Martin Space Systems Company
Speakers: David M. Keicher, Sandia National Laboratories
Edwin Schwalbach, Air Force Research Laboratory
Yu-Ping Yang, EWI

3:30 p.m. **Session 8: Additive Manufacturing Scalability, Implementation, Readiness, and Transition**
Facilitator: Anthony DeCarmine, Oxford Performance Materials
Speakers: Rainer Hebert, University of Connecticut
Alonso Peralta-Duran, Honeywell International Inc.
Tahany El-Wardany, United Technologies Research Center

5:15 p.m. **Adjourn Day 2**

DAY 3: OCTOBER 9, 2015

8:30 a.m. **Session 9: Reflections**
Theoretical Understanding of Materials Science and Mechanics
Facilitator: Steve Daniewicz, Mississippi State University

Computational and Analytical Methods in Additive Manufacturing
Facilitator: Wing Kam Liu, Northwestern University

Monitoring and Advanced Diagnostics to Enable Additive Manufacturing Fundamental Understanding
Facilitator: Jian Cao, Northwestern University

Additive Manufacturing Scalability, Implementation, Readiness, and Transition
Facilitator: Anthony DeCarmine, Oxford Performance Materials

10:00 a.m. **Session 10: Closing Session**
Facilitators: Wing Kam Liu, Northwestern University
Anthony DeCarmine, Oxford Performance Materials

12:00 p.m. **Adjourn Workshop**