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Born Qualified Grand Challenge LDRD Final Report

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Abstract

This SAND report fulfills the final report requirement for the Born Qualified Grand Challenge LDRD. Born Qualified was funded from FY16-FY18 with a total budget of ~$13M over the 3 years of funding. Overall 70+ staff, Post Docs, and students supported this project over its lifetime. The driver for Born Qualified was using Additive Manufacturing (AM) to change the qualification paradigm for low volume, high value, high consequence, complex parts that are common in high-risk industries such as ND, defense, energy, aerospace, and medical. AM offers the opportunity to transform design, manufacturing, and qualification with its unique capabilities. AM is a disruptive technology, allowing the capability to simultaneously create part and material while tightly controlling and monitoring the manufacturing process at the voxel level, with the inherent flexibility and agility in printing layer-by-layer. AM enables the possibility of measuring critical material and part parameters during manufacturing, thus changing the way we collect data, assess performance, and accept or qualify parts. It provides an opportunity to shift from the current iterative design-build-test qualification paradigm using traditional manufacturing processes to design-by-predictivity where requirements are addressed concurrently and rapidly. The new qualification paradigm driven by AM provides the opportunity to predict performance probabilistically, to optimally control the manufacturing process, and to implement accelerated cycles of learning. Exploiting these capabilities to realize a new uncertainty quantification-driven qualification that is rapid, flexible, and practical is the focus of this effort.

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NOMENCLATURE

Abbreviation	Definition
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AM	Additive Manufacturing
DED	Discrete Element Dynamics
ICME	Integrated Computational Materials Engineering
KMC	Kinetic Monte Carlo
LENS	Laser Engineered Net Shaping
MD	Molecular Dynamics
P-S-P-P	Process – Structures – Properties - Performance
SLM	Selective Laser Melting
TRL	Technical Readiness Level

1. INTRODUCTION

Additive Manufacturing (AM) is a flexible, agile production pathway ideal for low volume, high value, high consequence, complex parts that are common in high-risk industries such as defense, energy, aerospace, and medical [1,2]. To achieve a paradigm shift in qualification using the promise of AM there are multiple technical challenges that must be addressed. Today, AM processes suffer from challenges with variability in part quality due to build-to-build inconsistencies, inadequate dimensional tolerances, surface roughness, grain size, and defects [3, 4]. These challenges result in costly and time consuming post-build processes (e.g. Hot Isostatic Pressing, machining) to inspect/remediate internal defects (porosity, cracks), alter material properties (strength, ductility), or introduce surface modifications (finish, tolerance). Minimizing these added post-build processes is strongly desirable for financial and qualification needs. Having the ability to predict properties, structure, and performance of AM builds allows for the use of optimization for part performance and the ability to eliminate -- or at least reduce -- post-build processing to specific locations known before the build.

Inherent to the paradigm shift needed to change qualification is the integration of computational and physical models that comprise of a range of material options and incorporate multiple length and time scales. Utilizing these integrated models to produce a validated, predictive capability integrated with real-time and ex-situ diagnostics is the foundation of this approach. The technical challenges to achieve this new paradigm can be divided into five key areas.

1. Novel real-time AM diagnostic tools to quantify and monitor critical AM process variables for materials control and optimization.
2. Innovative and rapid experimental techniques to calibrate and validate models as well as correlate materials performance to in-process diagnostic measurements.
3. Computational models to relate process conditions to microstructure and ultimately to bulk measurable properties.
4. Approaches to characterize, model, and control variability in AM processes.
5. Intelligent data collection from various and diverse sources to develop science-based heuristics.

The need to bridge multiple length and time scales is intrinsic in these technical challenges, which favors an approach that is hierarchical, optimization focused, and science-based. The acquisition of foundational knowledge through novel real-time AM diagnostics [5] and materials assessment techniques ultimately progresses to next-level assemblies and then to full component qualification.

A new qualification approach is motivated by using AM to advance component design [6] and performance. Tight control of the manufacturing process promotes the ability to increase process yields and fosters the ability to predict process performance. Materials can be designed with desired properties for performance while facilitating easier characterization of property measurements for model calibration. Designing model validation experiments for the expected material and component performance provides a direct line to mechanistic model-form development and performance assessments. These validated models elucidate the Process-Structure-Property-Performance (P-S-P-P) connectivity that is difficult or impossible to deduce

experimentally. Validated computational models require extensive experimental observations to understand the domain of model agreement or bias and uncertainties in model predictions. Ultimately, as highlighted in Figure 1, using the capabilities of AM integrated with a validated, predictive capability and real-time and ex-situ diagnostic tools facilitates creation of a framework to translate AM Process results to material properties by relating micro Structure to bulk measurable Properties to ultimately predict component Performance.

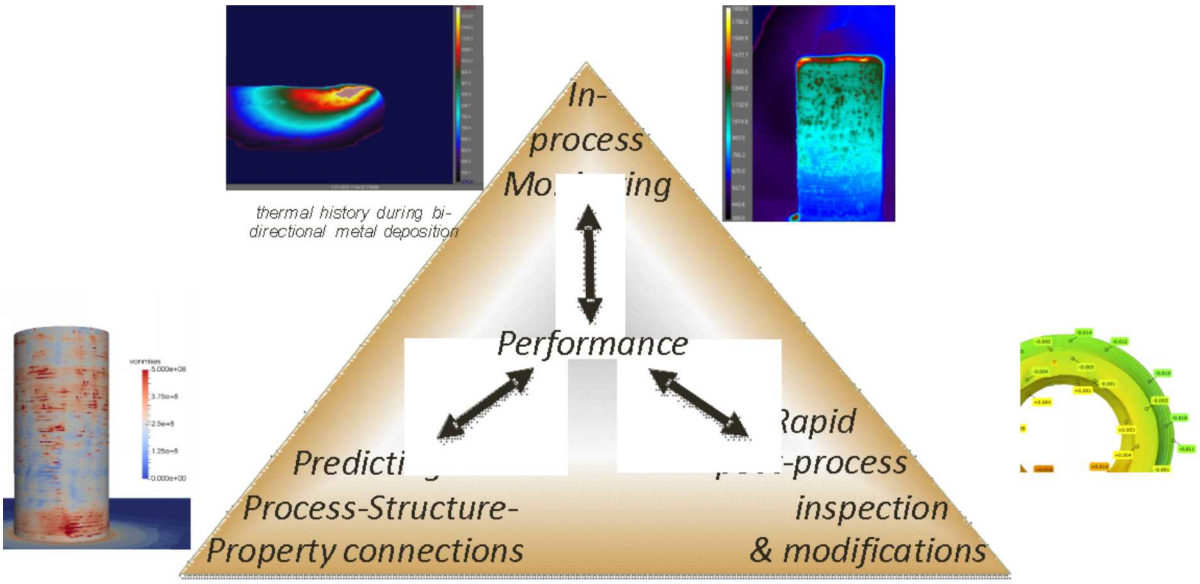


Figure 1: General P-S-P-P approach to development of a New Qualification Paradigm

Another driver in the development of a new qualification paradigm using AM is the ability to decrease the length of the product cycle from design through production. This is especially true for high value, high consequence, complex parts common in high-risk industries where requirements for high reliability often leads to cost inefficiencies, loss of flexibility, and diminished agility in designs. Figure 2 shows a notional construct of how a reduction in cycle time can be achieved. The first reduction, Figure 2b, is in time-to-build using the inherent promise of AM to quickly produce parts and components. A second reduction, Figure 2c, is tied to the ability to predict component performance, greatly reducing the dependence on validation tests of process and performance. These cycle time reductions are partially driven by an expansion of the design phase [7] to allow for a focus on prototype development. Advanced prototyping supports an Accelerated Cycle of Learning [8] approach, where confidence and knowledge is increased with more information available earlier in the product cycle. Overall the improved cycle time is a natural output of using AM to enable probabilistic performance estimation, design optimization, and P-S-P-P connectivity, which are all key requirements to creating new performance regimes for changing design, manufacturing, and qualification.

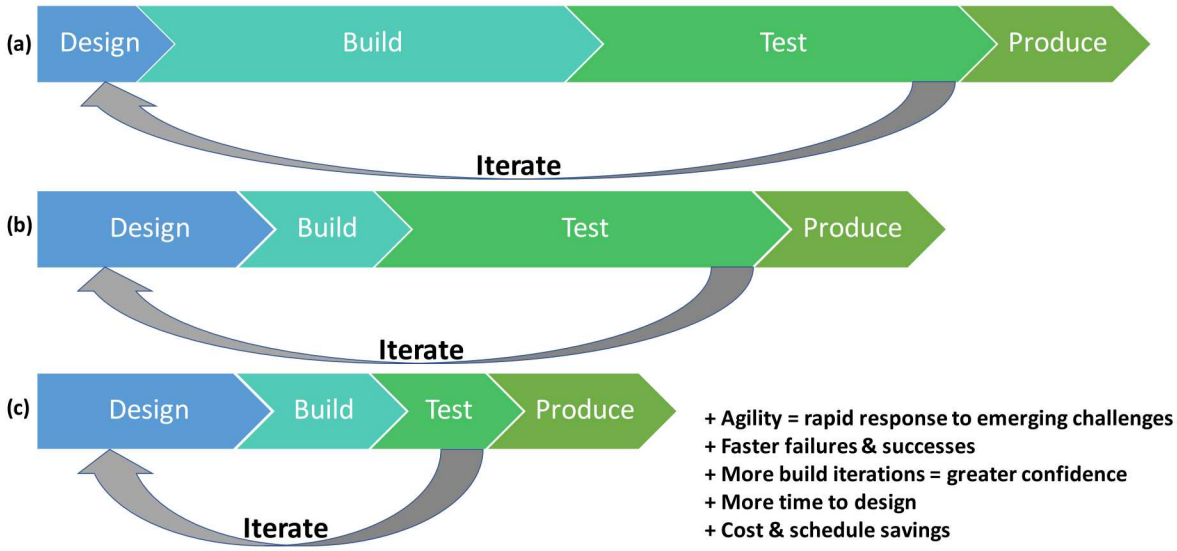


Figure 2: Overview of an improved a product cycle to achieve New Qualification Paradigm, (a) typical product cycle using traditional manufacturing processes, (b) product cycle using AM capabilities, (c) product cycle possible using AM with ability to predict performance

1.1. Implementation and Organization

The development of a new qualification paradigm that is rapid [9], flexible, and practical centers on developing a validated, predictive capability via integrated models in conjunction with real-time in-process and ex-situ diagnostics. The technical challenges that must be overcome to achieve the new paradigm will be discussed in the following sections. This paper is organized by focusing on the core technical challenges to achieve a new qualification paradigm. Process in-situ diagnostic needs, performance benchmark artifacts, and need for capabilities to rapidly characterize materials are discussed in **Assessing Materials and Process Performance**. Modeling and simulation needs to bridge the time and length scales, the need for P-S-P-P connectivity, and the capability to predictive performance is discussed in **P-S-P-P Models**. How data science and optimization is at the heart of the challenge to develop the new qualification paradigm is overviewed in **Optimization and Uncertainty Quantification**. Explorations into developing new and novel materials and structures are introduced in **Novel Materials and Structures**. Each of the topics sections in each chapter will begin with an overview of the scope of work followed by more information on specific topics with highlights on Top 5 Accomplishments and selected Papers and Presentations.

We had four External Advisory Board meetings for Born Qualified. Each meeting was 1.5 days in length and resulted in a formal report of assessments and recommendations that was instrumental in plotting the path forward for our project. These four formal reports are contained in Appendices A through D.

2. ASSESSING MATERIALS AND PROCESS PERFORMANCE

Accurate performance predictions are essential for developing a viable qualification paradigm and require accurate and timely evaluations of the AM process and the materials produced. One of the most significant technical gaps is the need for consistent and accurate measurement tools for in-situ diagnostics of the AM process [10,11]. In-situ measurements are the first step to quantifying and monitoring critical AM process variables for materials control and optimization, and providing correlation to the relevant physics of the process. New and novel measurement techniques, sensors, and correlations to materials science phenomena are needed, and must be well-suited to the spatial, temporal, environmental and processing considerations of AM. Real-time, in-situ measurements are also critical to developing a deep understanding of the AM process, with immediate determination of the impact of a requirement or manufacturing process change, while also allowing for changes in component performance to be quickly diagnosed.

Process control is impeded by a lack of adequate process measurement methods to characterize temperature, geometry, chemistry, phase content, and physical abnormalities, and to quantify and monitor critical AM process variables for materials control and optimization. The highly dynamic nature of some additive processes, e.g. laser powder bed fusion, introduces additional challenges as critical physical events can occur at time scales faster than sensor capabilities and length scales below typical sensor resolutions. Moreover, challenging subsurface measurements are desirable as the voxels continue to evolve and do not reach their metastable end state until they are deeply buried below additional material.

Data management has been observed to be another barrier as high bandwidth process and sensor sets can quickly approach terabytes of data. Ideally, the assessment techniques would be able to define all relevant structure, chemistry, defects, and properties in every voxel of an additively manufactured material, with the goal of connecting all possible variables to part performance. The identification of benchmark process and performance artifacts are vital to materials characterization efforts and testing. Achieving a system that integrates the in-situ and process measurements with these benchmark artifacts would provide designers and process engineers a perfect storm of information for process control.

Accurate performance predictions are essential for developing a viable qualification paradigm, and AM provides a range of possible options including uniquely designed benchmark process and performance artifacts, and the use of exemplars to demonstrate efficacy of the approach. These artifacts can be designed to provide accurate validations of performance predictions and monitor process stability. While process and performance artifacts ideally will be identical, it is noteworthy to differentiate between process verification and component performance. Process artifacts (e.g. sacrificial specimens) are typically used to verify process performance through a post-process evaluation. The selection of artifacts for process control and evaluation is a well published subject [12,13] and these efforts are guides to select appropriate performance artifacts.

Performance artifacts in our new qualification paradigm have the goal of verifying component performance in conjunction with in-situ manufacturing diagnostics and predictions of performance. Overall these performance predictions would ideally change the purpose of post-

process, product testing to validation rather than performance evaluation. The selection criteria for the performance artifacts are driven by multiple requirements and constraints of AM. First, they must provide the ability to evaluate several material types to assess unique material, design, and process challenges. They should also have modest performance requirements to simplify testing requirements where preferably performance can be assessed by measuring a limited number of requirements, metrics, or properties. These performance artifacts must also be selected considering AM's strengths and shortcomings, such as dimensional tolerances or surface finish, that could dilute the focus from the goal. It also is reasonable to consider applications with an opportunity to evaluate the enhanced functionality of components which can be uniquely enabled by AM.

To succeed in AM material assessment, where properties might vary from voxel-to-voxel or build-to-build, the existing materials assessment paradigm must be modified. Conventional materials assessment typically requires time scales on the order of weeks to months to machine test coupons and prepare for chemical and metallographic microstructural analysis, relying on expensive and time-intensive non-destructive evaluation such as CT scans. The challenge is to create a rapid characterization capability to generate a material assessment in a matter of hours rather than months. A combination of high-throughput, rapid screening characterization techniques with more selective, higher-fidelity assessment of P-S-P-P connectivity using conventional methods is an ideal solution to characterize process variables at the needed spatial and temporal scales.

2.1. Topic Area: Millimeter-Wave Radiometry

2.1.1. Description: What it is, why it is important to AM and SNL, what are the challenges

Accurate measurement of absolute temperature and cooling rates during additive manufacturing processes has proven elusive, yet would provide unprecedented knowledge and control over a build. Determination of temperature using non-contact methods has numerous challenges, including variation in emissivity with temperature, wavelength, composition, oxidation, and surface roughness, among other factors. Temperature measurement in AM systems is further complicated by large dynamic temperature ranges and extremely dynamic thermal histories. Temperatures measured using infrared thermographic cameras in relatively simple builds have been shown to be off by hundreds of degrees Celsius.

We have designed, built, and tested a novel dual-receiver millimeter wave radiometer system operating at 137 GHz for measurement of temperature and emissivity from passive microwave emission. The approach offers several inherent advantages compared to infrared thermography, including extreme dynamic range (millions of Kelvin vs. a few hundred Kelvin for thermographic cameras), linear response as a function of temperature, and the ability to measure emissivity in-situ and real time using thermal return reflection measurement. The system is capable of measuring emission at stand-off distances using parabolic focusing mirrors. Some challenges remain, including 1) need for improved evaluation of temperature effects on transmission and reflection in optical systems, 2) better assessment of uncertainties from dynamic effects in the build and the melt, 3) improved acquisition rates (possible through increasing the measured frequency to the THz-wave regime), and 4) enhanced spatial resolution.

2.1.2. Top five things that we accomplished:

1. Designed and built a custom high-temperature furnace for melting prototypic AM materials.
2. Designed, built, and tested a first-of-a-kind custom dual-receiver millimeter wave radiometer system operating at 137 GHz for measurement of temperature via passive microwave emission.
3. Implemented a thermal return reflection (TRR) capability for determining emissivity real time, in-situ from reflectance measurements.
4. Designed and implemented a novel optical system for transmitting mm-wave radiation using parabolic mirrors in place of waveguide systems.
5. Developed key insight into effects of surface roughness and topography of additively manufactured parts on infrared emissivity.

2.1.3. Top papers/presentations/intellectual property

1. R. Murphy, E. Forrest, J. Stanford, P. Woskov. "Calibration and Characterization of a Dual Millimeter-Wave Receiver High Temperature Measurement System." *Review of Scientific Instruments*. (In preparation)
2. S. Taylor, E. Forrest, J. Stanford. "Investigating Surface Roughness Effects on Emissivity for Metal Additive Parts." Annual International Solid Freeform Fabrication Symposium. Austin, TX. August 13-15, 2018.
3. J. Stanford, R. Murphy, and E. Forrest. "Microwave Thermal Analysis and Calibration for Additive Manufacturing." NCSLI 2017 Workshop & Symposium Exhibition. National Harbor, MD. August 14-17, 2017.
4. R. Murphy, E. Forrest. "A Review of In-Situ Measurements for Additive Manufacturing Technologies." *Proceedings of the NCSLI 2016 Workshop & Symposium Exhibition*. July 2016.
5. R. Murphy, E. Forrest, P. Woskov, J. Stanford. "Passive Millimeter Wave Radiometer System for Calibration of Infrared Cameras." US Patent Application #16058855. August 8, 2018.
6. R. Murphy, E. Forrest, P. Woskov. "Passive mm-Wave Radiometer System for Calibration of Infrared Cameras." Sandia National Laboratories Technical Advance, SD #14475. August 13, 2017.

2.2. Topic Area: Alinstante

2.2.1. Description: What it is, why it is important to AM and SNL, what are the challenges

Figure 3 shows a rapid testing configuration [14] where an array of miniature tester bars is produced and tested using AM at a cost and time scale comparable to the testing of a few conventionally produced and tested tensile bars. Having the capability to print and test arrays of tensile bars provides a wealth of data quickly that allows for the capture of the statistical nature of many mechanical properties that is critical to the creation of a new testing paradigm that we refer to as "Properties *Alinstante.*" This testing paradigm requires high-throughput, real-time measurements used in tandem with more detailed, lower throughput measurements to efficiently establish the structure, process, and property relationships of AM materials. Innovative experimental techniques are essential to provide assessment of materials performance and properties, and are required to link the limited information available from *in-situ* information and process and performance artifacts to the full P-S-P-P relationships of real components [15].

(a) *(b)*

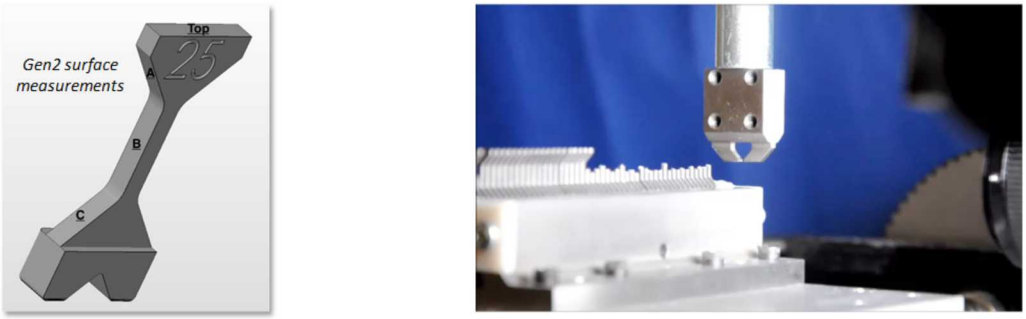


Figure 3: Rapid testing configuration for determining mechanical properties and performance. (a) shows the general mini-tensile bar geometry (b) is a picture of a rapid testing configuration for arrays of AM printed mini-tensile bars

Some quantities of interest in materials assessment are amenable to high-throughput automation and integration (e.g. hardness, chemistry, and electrical conductivity) whereas others (e.g. grain structure, long-term corrosion resistance, thermal diffusivity) are currently not. "Properties *Alinstante"* is required to link the information available *in-situ* (i.e. during processing) with complementary detailed structure and property measurements using conventional techniques to fully establish P-S-P-P relations. To this end, high-fidelity microstructural characterization is required to inform and calibrate multi-scale modeling techniques (including continuum, phase-field and molecular dynamics simulations) to provide microstructural information that can be referenced performance. The ability to predict process and component performance is the first step towards design-by-predictivity.

Our goal was to develop rapid post-build approaches to inspection, qualification, and model validation. While the AM process accelerates build times, subsequent assessment and

qualification has not yet been accelerated. To develop confidence in in-process metrics and validate model predictions for qualification, it is necessary to have complementary high-throughput automated inspection techniques. Building on our prior experience in high-throughput tension testing, we teamed up with Robotics experts to develop the *Alinstante* workcell with an integrated 3D scanner module. The scanner has the ability to collect as many as 1 million unique point cloud measurements within ~3 minutes to assess the geometric compliance of the part, and can be used for post-build inspection, or also inspection after subsequent process such as heat treatment or hot isostatic press. It was used to inspect the Insulator Ring exemplar as well as other Born Qualified related printed parts. The flexibility of *Alinstante* will allow us to add additional modules to meet the needs of future customers. In addition to the *Alinstante* workcell, our team explored the development of diagnostic artifacts and the use of high-throughput analysis to identify rare weakest-link failure modes.

2.2.2. Top five things that we accomplished:

1. Developed and submitted a patent application for a flexible robotic workcell (*Alinstante*), including sample handling, safe operation, control software, and queue management software. Integrated a 3D scanner into the *Alinstante* workcell, used to verify dimensional tolerances for additive components and witness coupons.
2. Broadly advertised the new *Alinstante* capability through a Sandia News Release, Youtube Video, and numerous trade journal articles. As a results, we have been in discussion with several companies including Fortune 500 companies who are potentially interested in *Alinstante*.
3. Developed first- and second-generation diagnostic artifacts. Unlike traditional test artifacts, such as the NIST artifact, we created artifacts for both verification of printability / dimensional tolerance, but also containing features suitable for material property measurement.
4. Developed a 2nd-generation high-throughput tensile system that is capable of up to 50 automated tests.
5. Used high-resolution in-situ tomography to explore the causal correlation between internal pore networks and fracture. Cluster analysis revealed that populations of proximate pores drive the failure process.

2.2.3. Top papers/presentations

1. B.C. Salzbrenner, J.M Rodelas, J.D. Madison, B.H. Jared, L.P. Swiler, Y-L. Shen, B.L. Boyce. “High throughput stochastic tensile performance of additively manufactured stainless steel,” Journal of Materials Processing Technology, 2017, vol 241, pp 1-12.
2. B.L. Boyce, B.C. Salzbrenner, J.M. Rodelas, L.P. Swiler, J.D. Madison, B.H. Jared, Y-L Shen. “Extreme-value statistics reveal rare failure-critical defects in additive manufacturing,” Advanced Engineering Materials, 2017, vol 19(8).
3. B.H. Jared, M.A. Aguilo, L.L. Beghini, B.L. Boyce, B.W. Clark, J. Robbins, “Additive Manufacturing: Toward Holistic Design”, Scripta Materialia, 2017.
4. [invited] B.L. Boyce, “Born Qualified? The challenge of qualifying additively manufactured metals for high-reliability applications”, University of California at Santa Barbara, CA, April 2016.

5. M.D. Uchic, B.L. Boyce, “Autonomy in Materials Characterization and Testing”, invited publication in preparation for MRS Bulletin, 2018.

3. P-S-P-P MODELS

A predictive, science-based description of the relevant mechanism responses for the observed properties in AM materials is the end goal for P-S-P-P connectivity. This requires predictive models to be developed using an Integrated Computational Materials Engineering (ICME) [16] approach to achieve fundamental physics-driven design from microstructure to parts and then components. Computational models must relate microstructure to bulk measurable properties to translate AM process results to predictable material properties and ultimately product performance. As such, the structure-property connections in AM materials must encompass the three main length scales: micro-meso material modeling, macro-modeling, and process modeling. Ultimately it is expected that validated computer models will guide the synthesis process, providing a feedback loop for selection of process parameters.

A modeling approach to bridge the length scales is shown in Figure 4 for a metal AM process such as a powder-bed fusion or Laser Engineered Net Shaping (LENS) process [17]. The overarching goal of this modeling technique is to eventually achieve finite element analyses of full parts, with accurate thermal histories, microstructures and residual stress fields. Such an approach requires input from all length scales of modeling. We begin with the mesoscale, where discrete element dynamics (DED) simulations are used to study the packing of powder particles [18] as they are spread across the substrate, as in a powder-bed fusion machine. Because the DED simulations have no inherent length scale, it is possible to construct atomistic

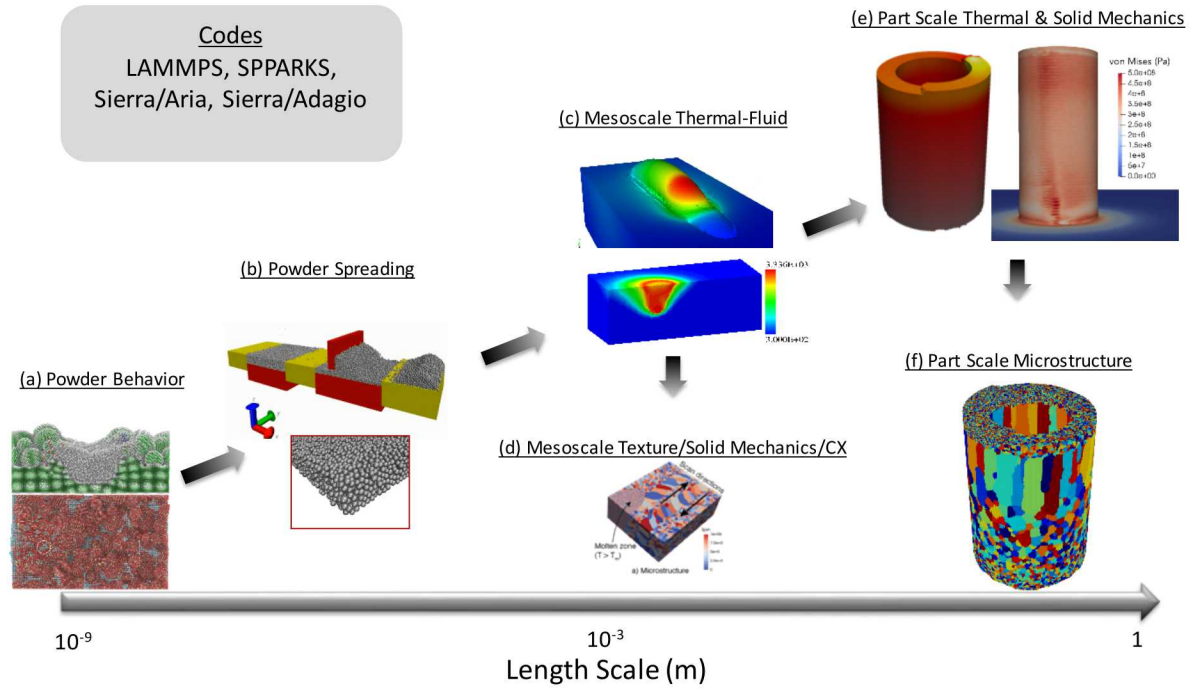


Figure 4: AM process is being simulated at multiple length scales. (a and b) At the powder scale, molecular dynamics and discrete element methods are used to study powder particle flow and physical properties. (c and d) At the mesoscale, combined thermal-fluid simulations provide detailed meltpool information and surface shape. Microstructure simulations also give insight to solidification grain structures. (e and f) At the macroscale, simulations of full parts provide thermal histories and residual stress fields, along with microstructural effects on part performance.

representations of the particles in the simulated powder pack, to study via molecular dynamics (MD). MD is used to determine the thermal conduction of metals in a powder bed environment, which will give accurate information about the size and shape of the melt pool as a function of laser power and beam width. It is also possible to use these simulations to study changes in melt pool geometry due to oxidization of powders, or powder packs that have skewed size distributions due to powder re-use. Melt pool geometries and thermal conductivities from mesoscale powder and process models are being imported into Kinetic Monte Carlo (KMC) simulations, along with thermal histories from macroscale simulations, to develop models of the unique microstructures found in metals subjected to a moving heat source. With accurate microstructures available, microstructurally-aware finite element analysis can be utilized to determine residual stresses in as-built parts [19]. The potential predictive impacts of the models are wide-ranging, and will require iterative loops of experimental characterization and modeling with applied mechanical and thermal stresses to determine feasibility [20]. These models may ultimately identify process routes presently outside the bounds of what is practical or achievable, and guide the design of next-generation AM systems.

3.1. Topic Area: Materials Models

3.1.1. Description: What it is, why it is important to AM and SNL, what are the challenges

The general goal for the materials modeling component of the Born Qualified grand challenge was to develop predictive modeling capabilities for materials during AM. Specifically, these models were to include atomistic and mesoscale details that are often overlooked in higher length scale models, such as chemical specificity and microstructural development. The primary focus was to determine to what degree these details impact material properties and therefore part performance.

Progress towards this goal involved two modeling approaches and simulation length scales, MD ($\approx 10\ nm - 1\ \mu m$) and KMC ($\approx 1 \mu m - 10\ mm$). Efforts were focused on a variety of aspects in AM processes, including thermal conductivity in powder beds, localized elemental segregation, scalability and sensitivity of the melt pool to process parameters, and predictive modeling of microstructural evolution in complex build geometries. Models at both length scales required overcoming significant challenges, the greatest being the development of customized simulation code.

3.1.2. Top five things that we accomplished:

1. Developed a multi-scale molecular dynamics model for thermal conduction in atomistic simulations of metal powder beds that includes electron heat transfer, providing a method for modeling laser powder bed fusion
2. Evaluated the effects of powder size and distribution on thermal conductivity in 304L stainless steel and 718 Inconel and quantified the impact of elemental segregation on material properties
3. Worked with optimization team to develop large scale sensitivity analysis for optimization of process parameters to achieve an ideal melt in laser powder bed fusion

4. Developed a sophisticated mesoscale model of microstructure formation in metal AM in SPPARKS and applied it to powder bed and LENS processes for a variety of materials.
5. Implemented a finite difference based thermal conduction model and directly coupled it with microstructural evolution, allowing for the simulation of complex build geometries with realistic boundary conditions.

3.1.3. Top papers/presentations

1. M. Wilson, M. Chandross, "Two-temperature model for thermal conductivity in alloyed metal nanoparticle powder beds," Draft in preparation.
2. M. Wilson, A. Kustas, M. Chandross, "Effects of grain size and elemental segregation during rapid solidification of metal alloys from atomistic simulations," Draft in preparation.
3. M. Wilson, K. Maupin, B. van Bloemen Waanders, and M. Chandross "Sensitivities for MD simulations," Draft in preparation for submission to *Additive Manufacturing*.
4. T.M. Rodgers, J.E. Bishop, J.D. Madison, "Direct Numerical Simulation of Mechanical Response in Synthetic Additively Manufactured Microstructures" Modelling & Simulation in Materials Science and Engineering 2018, 26(5)
5. T.M. Rodgers, J. Mitchell, V. Tikare, "A Monte Carlo model for 3D grain evolution during welding" Modeling & Simulation in Materials Science and Engineering 2017, 25(6)
6. T.M. Rodgers, J.D. Madison, V. Tikare, "Simulation of Metal Additive Manufacturing Microstructures Using Kinetic Monte Carlo" Computational Materials Science 2017, 135: p. 78-89
7. Presentations at Solid Freeform Fabrication Symposium 2016, 2017, 2018; American Physical Society 2017; Atomic Weapons Establishment-UK 2017, Gordon Research Seminar 2017, SIAM 2018

3.2. Topic Area: LENS Process Models

3.2.1. Description: What it is, why it is important to AM and SNL, what are the challenges

The overarching goal of this work is to use a multi-scale modeling approach to improve our understanding of how LENS process parameters affect part outcomes. At the mesoscale, we model the formation and behavior of the melt pool and directly account for incoming particle jet mass but do not resolve the individual particles. The width and depth of the melt pool dictate the catchment efficiency of the process as well as the amount of layer-by-layer remelted material. Detailed modeling of the transient temperature field and fluid flow within the liquid metal during a deposition allows for a better understanding of the effects of process parameters such as laser power and scan speed. While entire part builds cannot feasibly be modeled at this scale, information obtained from the model can provide significant insight and improve large scale reduced-order models.

In addition to mesoscale modeling, a macroscale Multiphysics finite element workflow was developed capable of modeling part scale LENS manufacturing. This workflow methodology was used successfully to model several different LENS builds that were also completed experimentally. Several cylindrical builds of the same geometry, but with differential laser scan patterns were simulated demonstrating the effects of laser scan pattern, and build plate size on the residual stresses. These results demonstrate that laser scan pattern could be used to engineer a residual stress state in a part during manufacturing. Additional improvements to robustness of this workflow have been made, and a 'lumped laser method' was implemented to help to improve computational speed without sacrificing fidelity in critical aspects of the build. Additionally, work has been conducted with UC Davis (PI: Prof. M. Hill) to make residual stress measurements of cylindrical LENS geometries and to validate model predictions. A primary limitation of this method is currently computational time required, which can be on the order of weeks for especially when simulating larger parts.

More recently, special attention was also given to focus on integration of the thermal/fluid model with the part-scale solid mechanics in Sierra/Aria and Sierra/SM to bridge length scales and improve fidelity. By tracking the surface topology changes for radiation and convection in SIERRA Aria, this new methodology provides a more accurate thermal history throughout the build. The resulting detailed thermal histories are then mapped over to a new mesh and used to inform the solid mechanics simulations, capable of predicting the evolution of residual stresses and microstructure within a part. This workflow might be used to propose optimal laser settings and process improvements by transferring information between scales.

Numerous challenges still remain, including 1) improvements in the robustness and efficiency of the coupled thermal/fluid and Sierra/SM model, 2) troubleshooting inconsistencies within the constitutive model and enhancements to melt physics (molten steel) in Sierra/SM, 3) calibration of the material fit to include high temperature (near melt) plasticity, 4) continued validation of the residual stress predictions with experimental builds, 5) improving the coupling by determining which quantities of interest can best inform and improve lower fidelity part-scale models

3.2.2. Top five things that we accomplished:

1. Calibration of the thermal/fluid model using wall build data from our LENS machine. Validation comparisons show good agreement on deposit height between the model and the measurements, providing confidence in the model.
2. Development and implementation of a mesoscale thermal/fluid LENS model in Sierra/Aria. The model utilizes the conformal decomposition finite element method (CDFEM) to dynamically track the interface between the metal and its gas environment as mass, momentum, and energy are deposited throughout the build. The solid and fluid regimes within the part are modeled using a temperature-dependent viscosity function.
3. Improvements in the robustness and computational throughput of the part-scale models using a "lumped laser" method.
4. Validation of the cylinder builds with simulation results demonstrating the effects of variations in the laser scan pattern and base plate size

5. Design and implementation of a new workflow with improved fidelity for integration of the thermal/fluid model with the part-scale solid mechanics model to calculate residual stress distributions

3.2.3. Top papers/presentations

1. Stender, ME, Beghini, LL, Sugar, JD, Veilleux, MG, Subia, SR, Smith, TR, San Marchi, CW, Brown, AA and Dagel, DJ. "A thermal-mechanical finite element workflow for directed energy deposition additive manufacturing process modeling." Additive Manufacturing 21, 556-566.
2. Stender, ME, Beghini, LL, Sugar, JD, Veilleux, MG, Subia, SR. “Process Modeling of LENS Manufacturing: Effects of Laser Scan Path on Residual Stress”. World Congress of Computational Mechanics in NY, 2018.
3. Stender, ME, Beghini, LL, San Marchi, CW, Sugar, JD, Veilleux, MG. “Process Modeling of Additive Manufacturing for Structural Performance Predictions”. Structural Reliability Partnership Workshop in Boulder, CO.
4. B. L. Trembacki, D. R. Noble, S. R. Whetten, M.J. Martinez. “Thermal-Fluid Mesoscale Modeling of the LENS Additive Manufacturing Process.” Integrating Materials and Manufacturing Innovation (to be submitted).
5. B. L. Trembacki, D. R. Noble, D. J. Dagel, S. R. Whetten, M. J. Martinez. “High-fidelity Mesoscale Thermal/Fluid Modeling of the LENS Additive Manufacturing Process,” 147th Meeting of the Minerals, Metals & Materials Society. 2018

3.3. Topic Area: Powder bed process models

3.3.1. Description: What it is, why it is important to AM and SNL, what are the challenges

In selective laser melting (SLM), successive layers of metal powders are selectively melted with a laser in order to manufacture complex, (potentially) multi-material three-dimensional parts from metal powders, including parts which cannot be constructed by conventional subtractive processes. However, the coupled interacting physical phenomena at the powder particle scale (e.g., melting/remelting, capillarity, flow, solidification) are not fully understood, but are central to optimizing the SLM process for production of reliable parts. Coupled experimental and modeling studies are essential for a deeper understanding of the process - structure - property relationship. We developed a full-physics, 3D, powder-resolved SLM model using a specialized interface tracking Level-Set technique (CDFEM) with conformal representation of the liquid-metal/gas interface. This general framework allows the physics code to describe either weak or strong discontinuities across the interface, resulting in a powerful model to simulate the melting of powder particles and motion of the melt flow. We also developed an Sierra-based method to interpolate data for the kinetic Monte Carlo microstructure model to enable microstructure prediction based on the realistic dynamic powder bed simulations.

3.3.2. Five things that we accomplished:

1. The model was applied (prior to the availability of Born Qualified powder bed data) with steel powders and laser parameters relevant to Born Qualified to understand and study the impact of laser settings and powder morphology on surface finish, melt track shapes, part defects (pores, un-melted regions) and microstructures.
2. The powder bed model was applied for simulation of single track validation Born Qualified Demonstrator 1A experiments with varying laser power, scan rate, and powder packing density. Selected simulations were mapped for use with KMC for predicting microstructures.
3. Developed and applied UQ methods for flat plate and powder bed melting models using polynomial chaos expansions.
4. Completed UQ analysis for flat plate melt track shapes considering laser power, beam diameter and surface tension coefficients. Demonstrated ability of model to predict melt track shapes on flat plates to within calculated uncertainty.
5. Completed a UQ analysis of Demonstrator 1A for steel powder bed data. Model predictions of melt track shapes were found not to match data due to unmodeled uncertainties, additional challenges of powder bed models, and difficulties with experimental data. Effort is continuing as better data comes available. Nevertheless, the comparisons instill confidence in other model-predicted trends such as melt pool temperature and penetration depth. Comparison of microstructure is also being performed. Further calibrations and model improvements are needed to get better simulation comparisons with available data.

3.3.3. Papers/presentations

1. MJ Martinez & DR Noble, Modeling of Selective Laser Melting: Impact of laser settings and powder morphology, SAND2017-5814A, USACM-TMS Additive Manuf. conference in Golden, CO, 09/06/2017 - 09/08/2017.
2. Dan Moser, Bradley Jared, Joshua Koepke, and Mario J Martinez, Towards a Predictive Mesoscale Model of the Selective Laser Melting Process, Submitted to *Additive Manufacturing*, Elsevier, Sept. 2018.
3. Moser & Martinez,"Particle Scale Melt Modeling of Selective Laser Melting with Uncertainty Quantification," 2018 Solid Freeform Fabrication Symposium, August, 2018.
4. Theron Rodgers; Daniel Moser; John Mitchell; Fadi Abdeljawad; Mario Martinez; Kyle Johnson; Jonathan Madison, Simulating Microstructural Evolution from a Single Bead to (Closer to) the Part Scale, 29th Solid FreeForm Fabrication Symposium, Aug. 2018.
5. Ford, Johnson, Trembacki, Bishop, Martinez, Noble, Multi Scale Solid Mechanics Models of Additive Manufacturing, TMS, March 2018.
6. Ford,Kurtis Ross, Johnson, K., Bishop, JE and Martinez, Mario J., Consideration of Fluid Physics on the Residual Stress in a Singe Track of Material, SAND2017-4232A, Annual International Solid Freeform Fabrication Symposium in Austin, Texas, USA from 08/07/2017 - 08/09/2017.
7. K Ford, K Johnson, MJ Martinez, JE Bishop, An Overview of Solid Mechanics Additive and Weld Models at Sandia New Mexico, SAND2017-6955A, JOWOG 28, Reading, Berkshire, United Kingdom, 08/29/2017 - 09/01/2017.

8. MJ Martinez, 2018, Melt pool dynamics in additive manufacturing, ASC PEM Meeting, LLNL, 7-9 Feb.

3.4. Topic Area: Direct Write process Models

3.4.1. Description: What it is, why it is important to AM and SNL, what are the challenges

The direct write additive manufacturing process represents an enabling capability due to increased flexibility and versatility of shape and configuration over traditional sintering processes. Such additional performance does come at the cost of increased complexity of the inherently multiscale problem. Specifically, both microstructural characteristics of the direct write "ink" and macroscopic features of the write process must be understood and controlled. Individually, each scale poses a modeling challenge that requires improvements over existing capabilities. Appropriately describing the direct write process, however, needs a treatment that allows for the consideration of both scales simultaneously. It is only possible to leverage these capabilities in a design role if the various models are done in an efficient fashion.

To address these issues, a wholistic modeling campaign was undertaken at and across the relevant physical scales. Lower scale approaches were used for detailed investigations of the relevant physics and phenomena of the ink material while continuum constitutive and finite element analysis was used for consideration and analysis of the macroscale problem. Importantly, the results of mesoscale analyses were used to motivate constitutive forms thereby integrating the different scale and the various capabilities. Experimental characterization was also performed to augment results of the lower scale endeavors in developing appropriate constitutive descriptions. Taken together, such activities have advanced capabilities at each of the relevant scales and created an integration pathway for the modeling and analysis of the direct write process.

3.4.2. Five things that we accomplished:

1. Developed a new phase field-based, mesoscale modeling framework that includes both thermodynamic and mass transport contributions. The resultant model was used to study the impact of microstructure (e.g. particle size distributions) on the sintering response and kinetics.
2. Derived a new, thermodynamically consistent sintering stress form motivated by the results of the phase field model and incorporating a term related to particle size distributions.
3. Utilizing aforementioned phase field framework with a three-particle configuration, demonstrated the impact of the ratio of grain boundary to free surface energy on pore kinetics.
4. Characterized the strength of direct written bars in terms of processing parameters to inform/motivate a corresponding constitutive model.
5. Developed, implemented, and verified a new fully implicit integration scheme for continuum sintering models for use in finite element frameworks.

3.4.3. Papers/presentations

1. F. Abdeljawad, D. Bolintineanu, A. Cook, H. Brown-Shaklee, C. DiAntonio, D. Kammler, and A. Roach. "Sintering Processes in Direct Ink Write Additive Manufacturing: A Mesoscopic Modeling Approach," *Acta Materialia*, 2018, Submitted.
2. J. Sestito, F. Abdeljawad, T. Harris, and Y. Wang. "The Role of Grain Boundaries in Nanoscale Sintering: An Atomistic Simulation Study," *Acta Materialia*, 2018, Internal Review.
3. B. T. Lester, F. Abdeljawad, and J.E. Bishop. "A Sintering Stress Formulation Incorporating Particle Size Distributions", *Journal of American Ceramic Society*, 2018, Internal Review.
4. B. T. Lester. "Verification of the Skorohod-Olevsky Viscous Sintering (SOVS) Model", Memo, 2017, SAND2017-12933R.

3.5. Topic Area: Exemplar Models

3.5.1. Description: What it is, why it is important to AM and SNL, what are the challenges

A key aspect of current and future qualification efforts is accurate part-scale modeling and simulation. Predictive models can allow for margin and uncertainty quantification, as well as identify critical performance characteristics that are sometimes difficult or impossible to determine experimentally. Residual stresses are an example of one of these characteristics that are often present in AM parts. Before the Born Qualified GCLDRD, Sandia did not have a capability to model the AM process to predict phenomena such as residual stress. As a result, a significant effort was made to develop this capability. Though commercial codes now exist for this purpose, many were still in their infancy 3 years ago and to date still have many drawbacks, such as a lack of a physics. Often, these codes will be empirically calibrated to specific materials on specific AM machines, which does not align with the spirit of Born Qualified of developing a deep science-based understanding. To gain this understanding, physically-based part-scale thermal and solid mechanics models were developed within Sierra, Sandia's massively parallel finite element code. These models allow for the accurate simulation of each laser pass and build-up of parts in both the LENS and laser powder bed fusion, and fiber-fed processes. One of these models was used to predict the residual stress in a LENS-fabricated tube and published in paper 1 from the publication list in this section. After these full resolution models were completed, more computationally efficient reduced-order models were developed in order to simulate large builds that would be prohibitive using the full resolution models, such as the exemplar valve housing. The valve housing is over 1.3" tall, which equates to over 1100 print layers and over 6 hours of build time. The reduced order model was able to simulate this build in 24 minutes, which is over 14x faster than real time. The residual stress results of this model were compared to neutron diffraction measurements performed at Los Alamos National Laboratory and showed good agreement, as shown in Figure 5.

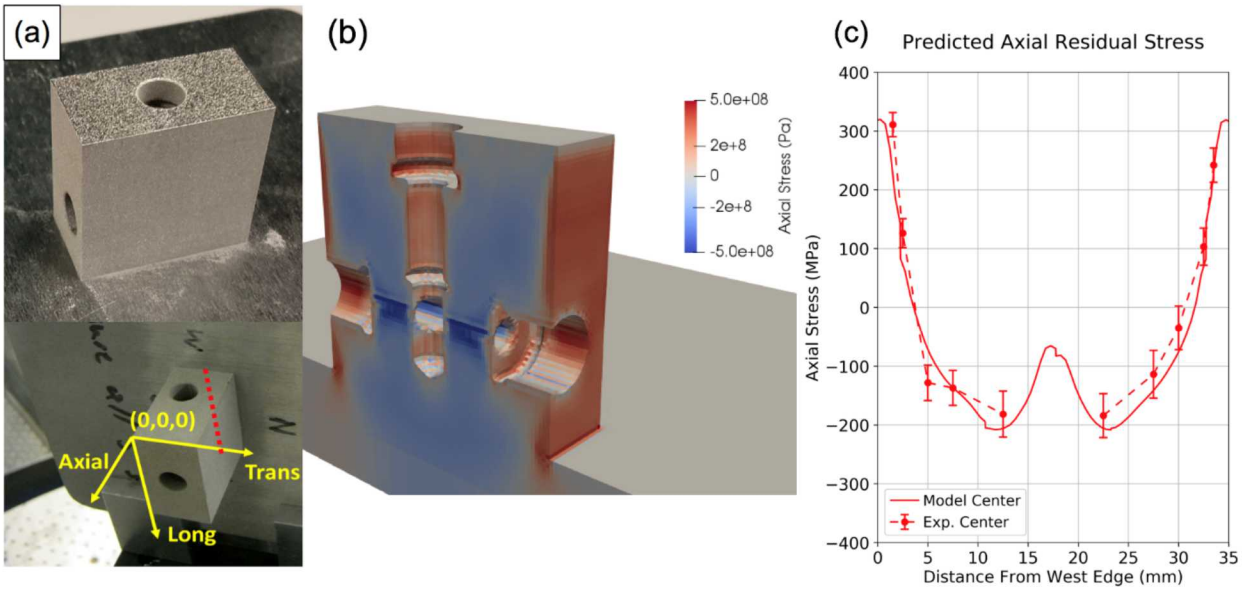


Figure 5. (a) As-built part and orientation during neutron diffraction (b) Mid-plane cut view of build direction residual stress prediction from Sierra showing interior compressive stress and external tensile stress (c) Comparison of experimental neutron diffraction residual stress results from LANL to model predictions along red dashed line in (a) showing good agreement.

Another important achievement of the Born Qualified effort was the coupling of Sierra thermal results with SPPARKS three-dimensional microstructure simulations. This coupling allowed for prediction of grain morphology evolution that is directly dependent on the thermal history that an AM part undergoes. This capability was used to show that process factors such as inter-layer delay times can cause significant changes in microstructure. Results of this capability were published in paper 1 from the publication list in this section.

Finally, a process was developed for including as-built properties into performance simulations. Specifically, the initial higher yield stress often present in AM materials can be captured and included in performance simulations. Porosity and defects were also accounted for by directly mapping them onto the mesh.

3.5.2. Top 5 Accomplishments

1. We developed full-resolution part scale process models for both LENS and laser powder bed fusion in Sierra to model the AM process, which was not possible before Born Qualified.
2. We developed an efficient, reduced order model for residual stress prediction that is faster than real-time printing.
3. We validated the valve housing exemplar residual stress state with neutron diffraction data from LANL
4. We developed the capability to transfer thermal results as input into SPPARKS to predict thermal history-dependent microstructure evolution.
5. We developed the capability to perform performance simulations using as-built properties and residual stress, with a method of mapping porosity or defects onto mesh in the form of damage

3.5.3. Top papers/presentations

1. Johnson, K.L., Rodgers, T.M., Underwood, O.D., Madison, J.D., Ford, K.R., Whetten, S.R. Dagel, D.J., and Bishop, J.E. “Simulation and Experimental Comparison of the Thermo-Mechanical History and 3D Microstructure Evolution of 304L Stainless Steel Tubes Manufactured Using LENS”, Computational Mechanics, 2018.
2. Salloum, M., Johnson, K.L., Bishop, J.E., Aytec, J.M., Dagel, D.J., van Bloemen Waanders, B., “Adaptive Wavelet Compression of Large Additive Manufacturing Experimental and Simulation Datasets,” Computational Mechanics, 2018.
3. 4 invited conference presentations
    a. ASME IMECE 2017
    b. Smoky Mountains Computational Science and Engineering Conference 2017
    c. Solid Freeform Fabrication Symposium 2018
    d. MS&T Annual Meeting 2018
4. 25 total conference presentations

4. OPTIMIZATION AND UNCERTAINTY QUANTIFICATION

Ultimately optimization, data science [21,22], and uncertainty quantification [23-26] are at the heart of our Born Qualified challenge. Overall the goals are to (1) use optimization as the interface between simulations, experiments, data, and uncertainties, (2) map numerical capabilities to real experiments, (3) use data science to ask questions, not just answer questions, and (4) use data science in each part of the P-S-P-P map. To provide maximum information and create robust solutions in the face of uncertainties, the development of a research strategy for intelligent data collection and analysis of diverse sources (experiments, diagnostics, models) requires generating, filtering, selecting, and sampling data. To transform practices, we need to be able to characterize uncertainties at all stages: at the raw material stage, during the AM process, in the resulting microstructure of the material created in the AM process, and ultimately, in the product created from that material. These uncertainties are characterized by enormous sets of experimental data, materials models across all length scales, and AM process models. Efficient techniques are needed to propagate parameter uncertainties through models, including sampling, stochastic expansions, interval analysis, and reliability methods. The ability to fully couple numerical multi-scale simulations with efficient analysis tools is necessary so that models can be calibrated, used in an optimal design process, and eventually guide the manufacturing process. Techniques must also be developed and implemented to calibrate model parameters with incorporated experimental uncertainty. Finally, we need to follow structured model validation processes [27,28] for comparing model predictions to experimental data and computing validation metrics under a variety of conditions. Validation helps ensure that each of the models shown in Figure 4 is appropriate for its intended use. This is necessary both for proper use of individual models and for the coupling of models across scales.

Materials characterization, "Properties *Alinstante",* experimental design, integration of AM modeling with micro-meso-macro scale modeling, optimal control, and risk-averse design optimization all play important roles in managing and characterizing uncertainties in the overall product development and qualification. These capabilities drive a possible framework for a new qualification paradigm shown in Figure 6. This new qualification framework utilizes a multi-scale approach that is rapid and flexible where performance is predicted probabilistically and the manufacturing process is tightly controlled. The computational and statistical methodologies exist to achieve end-to-end uncertainty quantification, but the integration with large data sets, many scales of material models, and preliminary AM models makes this task very challenging.

4.1. Topic Area: Uncertainty Quantification

4.1.1. Description: What it is, why it is important to AM and SNL, what are the challenges

To transform AM practices, we need to be able to characterize uncertainties at all stages: at the raw material stage, during the AM process, in the resulting microstructure of the material created in the AM process, and ultimately, in the product created from that material. These uncertainties are characterized by enormous sets of experimental data, materials models across all length scales, and AM process models. Efficient techniques are needed to propagate parameter uncertainties through models and calibrate model parameters by incorporating experimental data and its associated uncertainty. Finally, we need to follow structured model validation processes for comparing model predictions to experimental data.

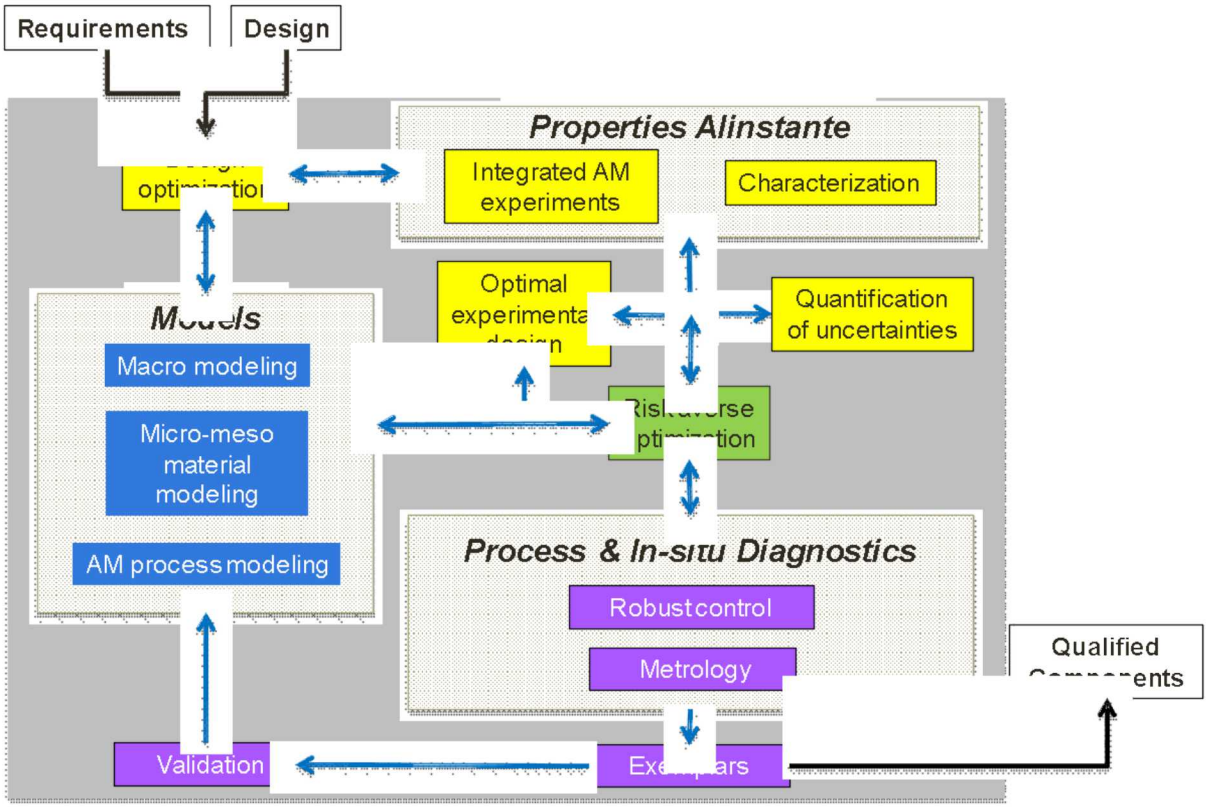


Figure 6: Framework for new AM-driven Qualification Paradigm

A major challenge in this project has been the lack of comprehensive data sets that covers all aspects: the manufacturing process, microstructure information, material properties of parts, and models at all levels that correspond to Process, Structure, Property, and Performance. For example, for our most comprehensive database of microstructure information (microCT scans on 100 tensile bars), we have no process information. Similarly, we have generated a large amount of tensile dogbones where we have process and property information but no microstructure information. Thus, most of the analysis has been relating only two or three elements of the P-S-P-P mapping. With that caveat, we have made significant advances in understanding the material variability resulting from AM processes and relating process variability to properties.

4.1.2. Five things that we accomplished:

1. 17-4PH Stainless Steel Powder-bed tensile bars: We generated spatial correlations showing the variation of material properties across the build plate, and used cluster analysis to map 15 material properties to 4 clusters of tensile bars with similar properties on the build plate. We developed stepwise regression models to relate porosity information from microCT scans (e.g. number of voids, average void size, average nearest neighbor distance) to yield strength.
2. 316L Stainless Steel Powder-bed tensile bars: Generated correlation analysis and regression fits to predict material properties (e.g. yield strength, ductility, cross-sectional area of the bar) with process parameters (laser power and scan velocity, radiant energy density). MicroCT data was very limited for these data sets, but showed that the material

properties of ductility, elongation, yield strength, and ultimate tensile strength did not appear to exhibit a trend with respect void metrics such as number of voids or average void volume. We performed a simulation prediction of yield strength with a coupled thermal/mechanical model of the powder bed process and compared this with experimental results.

3. 316L Stainless Steel AM process map for Powder-Bed machine: Based on experimental design, developed a process map relating laser power and scan velocity to identify optimal settings with respect to density and surface roughness of density cubes.
4. 316L Stainless Steel LENS process study: Used main effects analysis to identify significant differences in maximum melt pool temperature at two different power levels and plates scanned with and without powder. LENS build orientation study: used hypothesis testing and Weibull fits of yield strength with approximately 30 tensile bars each in three different orientations to identify a strongly significant effect of build orientation on resulting yield strength.
5. Direct Write: we had extensive data from the various aspects of the Direct Write process, including rheological properties of the feedstock, process parameters, and pre- and post-sintering data. We correlated voids from the green state CT with the pressure at the syringe tip (from the process) as a function of vertical layer in the build. We performed this analysis for an insulator ring and some demonstrator cubes. We also saw a significant effect of build orientation on yield strength for Direct Write.

4.1.3. Papers/presentations

1. B.C. Salzbrenner, J.M Rodelas, J.D. Madison, B.H. Jared, L.P. Swiler, Y-L. Shen, B.L. Boyce. "High throughput stochastic tensile performance of additively manufactured stainless steel," Journal of Materials Processing Technology, 2017, vol 241, pp 1-12.
2. B.L. Boyce, B.C. Salzbrenner, J.M. Rodelas, L.P. Swiler, J.D. Madison, B.H. Jared, Y-L Shen. "Extreme-value statistics reveal rare failure-critical defects in additive manufacturing," Advanced Engineering Materials, 2017, vol 19(8).
3. Tallman, A. E., Swiler, L. P., Wang, Y., and McDowell, D. L. "Reconciled Top-Down and Bottom-Up Hierarchical Multiscale Calibration of BCC FE Crystal Plasticity." International Journal for Multiscale Computational Engineering, 15(6):505–523 (2017).
4. Yan Wang (Georgia Tech) and Laura Swiler (SNL), co-editors of special issue: ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part B: Mechanical Engineering. Special Issue on Uncertainty Quantification in Multiscale System Design and Simulation. ASME J. Risk Uncertainty Part B. 2017; 4(1):010301-010301-2. doi: 10.1115/1.4037447
5. A. E. Tallman, K. S. Stopkab, L. P. Swiler, Y. Wang, S. R. Kalidindi, D. L. McDowell. "A Systematic Texture Effect Calibration in Polycrystalline Alpha-Ti." Draft in preparation for submission to Journal of Materials.
6. L. P. Swiler and K. L. Johnson. "Uncertainty Quantification for Additive Manufacturing Applications." TMS 2018 Annual Meeting, held March 12-15, 2018 in Phoenix, AZ. SAND2018-2654C.
7. K. Johnson, L.P. Swiler, T. Rodgers, B.H. Jared, S. Subia,K. Ford, M. Stender, J. Bishop. "Advanced Model Predictions of Mechanical Properties and Process Parameter Effects in

High Throughput L-PBF Tension Specimens." 2018 Solid Freeform Fabrication Symposium held August 13-15, 2018 in Austin, TX. SAND2018-8875C.

4.2. Topic Area: Optimization

4.2.1. Description: What it is, why it is important to AM and SNL, what are the challenges

The fundamental goal of the project was to achieve predictable material properties and performance by designing an optimal process control strategy. This entailed creating technology to find the best solutions that can accommodate a combination of constraints including process modeling, PDE-based numerical simulation, uncertainties, multiscale phenomena, and complex data. We focused on the development of large scale optimization, risk-averse methods, efficient PDE-based numerical simulation capabilities, risk-averse methods, multiscale simulation techniques, and sensitivity analysis for optimal control solutions. In particular, our development was centered around the needs of powered bed fusion, LENS, and Direct Write technologies. Each application motivated different challenges.

Numerous challenges needed to be addresses, consisting of developing 1) multi-scale capabilities, 2) efficient and flexible optimization techniques, capable of nonlinear dynamics as constraints, 3) numerical capabilities with adjoint and optimization interfaces, 4) methods to mitigate uncertainties in the context of a design criteria, and 5) methods to evaluate the importance of uncertain parameters in data and modeling.

4.2.2. Top five things that we accomplished:

1. Developed MILO with Mortar methods and multiscale optimization techniques
2. Enabled risk-averse optimization to connect design qualification specs, uncertainties, optimization and PDE-constrained optimization
3. Developed numerical control strategies to achieve temperature targets from pyrometers in a LENS process for 304L line scans
4. Implemented Peridynamics to simulate mechanical states for the green state, burn-off, and sintering process in Direct Write as a foundational capabilities for inversion and control
5. Developed intrusive and large scale sensitivity methodology to evaluate the priority of uncertain parameters in the dynamics in the context of optimal solutions

4.2.3. Top papers/presentations

1. T. Wildey, B. van Bloemen Waanders, and D. Seidl "Mortar methods"
2. H. Li and B. van Bloemen Waanders "Risk-averse optimization for atmospheric transport"
3. J. Hart and B. van Bloemen Waanders "Sensitivity analysis
4. A. Hegde, B. van Bloemen Waanders, D. Littlewood, S. Silling, H. Brown-Shaklee, and A. Cook "Peridynamics for direct write"
5. M. Wilson, K. Maupin, B. van Bloemen Waanders, and M. Chandross " Sensitivities for MD simulations

6. “PDE-constrained optimization” special journal edition OPTE, associated editors: M. Ulbrich and B. van Bloemen Waanders.
7. Presentations at SIAM C&E 2017, SIAM Opt 2016, 2018. TMS Annnual 2017, Copper Mountain Iterative Methods.

5. NOVEL MATERIALS AND STRUCTURES

As we develop the capabilities to assess and predict performance of the AM process, opportunities arose to also begin looking at the new materials and structures that were possible. These metamaterials are crucial to future exemplars and development efforts to fully utilize the unique capabilities of AM. The two areas of focus for Born Qualified were novel materials and lattice structures.

5.1. Topic Area: Novel alloy development

5.1.1. Description: What it is, why it is important to AM and SNL, what are the challenges

AM presents a unique opportunity to enable processing of ideal metals and alloys with unprecedented properties, a combination that is otherwise not achievable with conventional manufacturing technologies. In turn, these AM-enabled high performance materials will foster the development of next-generation devices with superior performance metrics and greater safety margins than current devices used in high consequence applications. We demonstrated this approach by applying state-of-the-art metal AM processes with soft ferromagnetic alloys that cannot be produced commercially. AM enabled favorable microstructures in specimens resulting in exceptional properties.

Some of the primary challenges of this effort include: (1) procurement of the ideal material powder, (2) optimization of process-structure-properties relationships, and (3) increase TRL to produce part-scale geometries for testing in lab environments. The powder materials where difficult to procure in a timely manner, challenging the timeframe for this work. Furthermore, the process demonstration and subsequent structure-properties characterization were proof-of-concept without quantifying uncertainty or variability. Finally, specimens were produced in test geometries only and not part-scale. While a significant amount of work remains to continue maturing this technology, important strides were made to demonstrate the potential of employing metal AM to enable novel or advanced materials design.

5.1.2. Top five things that we accomplished:

1. Go/no-go processing of Fe-Co and Fe-Si alloys at ideal compositions and in bulk form
2. Characterized preliminary process-structure relationships of these materials with opportunities to tune microstructures via the process parameters
3. Characterized mechanical and magnetic properties of bulk AM structures and determined tradeoff opportunities in performance
4. Identified an apparent trend in atomic ordering with respect to process cooling rate and thermal gradient data
5. Printed large-scale structures without significant defects or cracking

5.1.3. Top Papers/Presentations

1. A. B. Kustas, et al., *Characterization of Fe-Co soft ferromagnetic alloys processed by Laser Engineered Net Shaping*, Addit. Manuf., May 2018, p. 41-52, https://doi.org/10.1016/j.addma.2018.02.006
2. A. B. Kustas, et al., *Overcoming strength-ductility limitations in intermetallic alloys through additive manufacturing*, planned submission to Nature Materials or Advanced Materials
3. A. B. Kustas, et al., *Novel Processes and Materials Solutions for Metal Additive Manufacturing*, Invited talk at 2018 THERMEC Conference, Paris, FR, July 8-13
4. A. B. Kustas, et al., *Additive Manufacturing of Soft Ferromagnetic Alloys using Laser Engineered Net Shaping*, 2018 SFF Symposium, Austin, TX, Aug. 13-15
5. A. B. Kustas, et al., *Processing of Fe-Co Soft Ferromagnetic Alloys using Laser Engineered Net Shaping*, 2018 TMS Conference, Phoenix, AZ, Mar. 12-15

5.2. Topic Area: Lattices

5.2.1. Description: What it is, why it is important to AM and SNL, what are the challenges

Architected structural metamaterials, also known as lattice or truss materials, provide opportunities to produce tailored effective properties that are not achievable in bulk monolithic materials. These topologies are typically designed under the assumption of uniform, isotropic base material properties taken from reference databases and without consideration for sub-optimal as-printed properties or off-nominal dimensional heterogeneities. However, manufacturing imperfections present throughout the lattices create significant variability in mechanical properties and part performance.

This study utilized an idealized unit cell topology consisting of five parallel struts loaded in a stretch (tensile) orientation to examine the impact of manufacturing heterogeneities on structural performance. The strut unit cells and reference monolithic tensile bars were manufactured using a direct metal laser sintering (also known as laser powder bed fusion) process in a precipitation hardened stainless steel alloy, 17-4PH, with minimum feature sizes ranging from 0.5-0.82 mm, comparable to minimum allowable dimensions for the process. Over 70 tensile tests were performed revealing that the effective mechanical properties of the strut unit cells were highly stochastic, considerably inferior to the properties of larger as-printed reference tensile bars, and well below the minimum allowable values for the alloy. Pre- and post-test non-destructive analyses revealed that the primary source of the reduced properties and increased variability was attributable to heterogeneous surface topology and commensurate reduction in effective load-bearing area.

5.2.2. Top five things that we accomplished:

1. Demonstrated that lattice struts can exhibit a tensile strength as low as 40% of the “bulk” material. The reduction in strength is attributed to size and build orientation.

2. CT inspection of the struts revealed large differences in part quality for horizontal struts compared to vertical struts. Since horizontal struts were unsupported, there were large deviations in cross-sectional (or load-bearing) area.
3. Structural mechanics analysis of the CT data highlighted increased stress concentrations throughout the horizontal struts while the vertical struts had fairly uniform stress distributions.
4. The increased amount of stress concentrations throughout horizontal struts resulted in the strength of horizontal struts being, on average, ~20% lower than vertical struts.
5. Additional CT data analysis showed that struts are generally smaller than designed.

5.3. Top papers/presentations

1. A. Dressler, E. Jost, J. Miers, D. Moore, C. Seepersad, B. Boyce "Heterogeneities Dominate Mechanical Performance of Additively Manufactured Metal Lattice Struts," In preparation.
2. Presentation at SFF 2018

6. SUMMARY AND CONCLUSIONS

AM provides the opportunity to develop a new qualification paradigm for materials and components by incorporating deep materials and process understanding. This requires integrating a validated, predictive capability with real-time and ex-situ diagnostics to realize uncertainty quantification driven qualification of design and processes. Success in executing a new qualification paradigm will result in a revolution of component engineering, design, and manufacturing. This new framework, shown in Figure 6, requires integrated models, in-situ and process diagnostics, the use of artifacts and exemplars, uncertainty quantification, all within an optimization focus. Impacts of the new qualification paradigm are far reaching and substantial. Immediate determination of the impact of a requirement or manufacturing process change will be possible with the ability to predict performance of the process, materials and component. The new paradigm will allow for problems or unexpected changes in component performance to be quickly diagnosed and propagated through the design-manufacture-sustainment chain to assess impacts to an entire enterprise. In addition, the ability to verify and predict process stability and eventually materials assurance allows for science-based and trusted manufacturing and an increased confidence in lifetime performance.

The Born Qualified GCLDRD has fulfilled all milestones and deliverables over its 3-year lifetime. The P-S-P-P linkages were demonstrated through demonstrators and exemplars which integrated the experimental characterization, part properties, and modeling activities. We developed a computational models, for example, to predict residual stress for the valve housing, melt pool temperatures for LENS, yield strength for the powder-bed dogbones, and sintering effects across scales for direct write. This project also impacted more than 70 staff, Post Docs, and students as we successfully executed our mission. More importantly Born Qualified also functioned as the integration path for the many AM projects and efforts. This integration function will be missed at Sandia.

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APPENDIX A: EXTERNAL ADVISORY BOARD REPORT #1

External Advisory Board Report
Meeting: March 2-3, 2016

Born Qualified Grand Challenge LDRD

Sandia National Laboratories

This report is presented to Rob Leland, Vice President and Chief Technology Officer (CTO) and Andy McIlroy (Director of Research Strategy and Partnerships) and to the Born Qualified Grand Challenge LDRD project team at Sandia National Laboratories (SNL) by its External Advisory Board (EAB), following the meeting of March 2-3, 2016 in Albuquerque, New Mexico. This was the inaugural meeting of the Born Qualified EAB.

I. Summary Feedback

Sandia has assembled an outstanding high-performance team to address an extraordinarily complex materials qualification problem over the long term. Both the 15-year vision and initial steps proposed for the three-year GC are bold and potentially transformative. The EAB reminded Sandia to keep the focus on the challenges of qualification and not on the additive manufacturing (AM) process, which remains but one of many methods to produce components that require qualification.

As discussed at length during the meeting and in the outbrief session, both the 15-year vision and the three-year project plan are in critical need of a roadmap that outlines where the overall effort is headed and where / how each aspect plugs in. Specific suggestions are provided in the body of the report below.

Overall, the board believes that the Born Qualified (BQ) team is addressing the right issues and has the talent required to make real progress. The initial scope is necessarily broad but will be funneled down to the best set of activities within the first year as dictated by the roadmap.

The EAB identifies overall data management as a risk in the project, and recommends that a capable data scientist should be added to the team.

The project clearly has direct relevance to the mission of its nuclear weapons sponsor, and Sandia has both unique needs and deep technical capabilities that it can bring to bear on materials assurance in advanced manufacturing. Both the difficulty of the problem and the scope of work that Sandia can pull together into a single multi-disciplinary efforts make this a project worthy of a national laboratory. The Lab's special strengths are judged to be in computational multiscale modeling of materials processing, microstructure-property relations, and structural mechanics, uncertainty quantification, and materials science.

While it is clear that Sandia approaches its work with a high degree of scientific integrity, it is too early for the EAB to offer meaningful comments. The specific technical goals are not yet clear enough and need to be laid out in the roadmap.

The researchers working on the project all appear to be high caliber, and the EAB was particularly impressed with the early career staff.

On the question of partnerships, the board emphasizes that this should be part of the initial research that goes into the roadmap. All members emphasized that Sandia has "open access" to capabilities available at their institutions.

This project will have impact if it can determine what defines qualification and where it can be inserted into a manufacturing process. The ultimate BQ goal will take a long time to achieve, but much can be spun off as it is learned. It is also important to demonstrate interim wins to maintain the long-term support of sponsors.

II. Board Members

Members Present

- **Craig Blue**, EAB Chair, Chief Executive Officer, The Institute for Advanced Composites Manufacturing Innovation (IACMI) and Director, Advanced Manufacturing Office and the Manufacturing Demonstration Facility, Oak Ridge National Laboratory
- **Slade Gardner**, LM Fellow, Advanced Manufacturing & Materials, Advanced Technology Center, Lockheed Martin Space Systems Company
- **Elizabeth Holm**, Professor of Computational Materials Science, Carnegie Mellon University
- **Daryl Landeg**, Chief Technologist, Atomic Weapons Establishment (AWE), UK
- **David L. McDowell**, Executive Director, Institute for Materials, Regents' Professor and Carter N. Paden, Jr. Distinguished Chair in Metals Processing, Georgia Institute of Technology
- **David McMindes**, Chief Technology Officer, National Securities Campus, Honeywell Federal Manufacturing & Technologies, LLC. (FM&T)
- **William Tredway**, Leader, Advanced Manufacturing Technology, United Technologies Research Center

III. Charge to the EAB

The Board was provided with a set of questions to guide its evaluation of the project as presented. These are given below.

Research Assessment Elements and Focus Questions	
Strategy *Research strategy is clear, having strategic goals, areas of research focus, competitive analysis, and measures of success.*	Sandia has established a 15-year vision to fundamentally change the engineering design and qualification paradigm in the design and manufacture of nuclear weapons components using additive manufacturing (AM) techniques . The 3-year Born Qualified LDRD Grand Challenge is the first step toward this vision. • Is this vision bold and potentially transformative in the field of AM? • Do the goals of the BQ-GC project support this vision? Is the research strategy well planned, and is it focused on the right areas? • Is the scope of the project reasonable; should it be enhanced or diminished in specific areas to provide a more effective outcome? • What are the greatest technical risks; is the payoff appropriately high?
Relevance *Research enables the Labs' national security missions, benefits Sandia, DOE/NNSA, and the nation.*	• Is Sandia uniquely qualified to undertake this work; is it "National Lab-worthy?" • Where do you see the BQ Grand Challenge having an advantage over other efforts in the field?
Quality *Research is high quality and at the leading edge, and is performed with high integrity and fidelity.*	• Are the technical goals clear, and are they matched to the right problems? • What aspects of the planned research are leading edge?
Workforce / Capabilities *Research enables the attraction, retention and development of Sandia's technical staff, and the development of differentiating capabilities.*	• Do you see skill gaps in science / technology /engineering that need to be closed during the course of the project (i.e. through partnerships or hiring)? • Will this project serve to strengthen Sandia's technical base; in particular through opportunities offered to early career staff?
Impact *Research leads to outcomes supportive of strategic goals, such as S&E leadership, technology deployment and intellectual property.*	• Does the GC have an effective plan to engage with the broader community? • What would you anticipate to be the GC's long-term S&T legacy?

IV. Meeting Logistics

The EAB review session was held on Wednesday and Thursday, March 2nd and 3rd, 2016 at Sandia's main campus in Albuquerque, NM. On Wednesday, Andy McIlroy welcomed Sandia's guests, presented the Charge to the EAB, and gave an overview of SNL's LDRD program. Terry Aselage, Director Champion for the project, provided opening remarks and Allen Roach, Project Investigator, outlined the project's background, approach, and objectives. These talks were followed by a series of detailed technical presentations from GC team leads and a poster session. The board then met in a closed session, during which EAB members discussed their impressions of material presented throughout the first day.

The second half-day session on Wednesday, March 2nd, began with a brief recap of the first day, followed by additional technical presentations, a wrap up, and general discussion. The board then conducted a final executive session and presented its preliminary findings in an outbrief to SNL management and the BQGC team. The meeting concluded following questions and group discussion.

An agenda detailing talk titles and presenters is attached at the conclusion of this report.

V. EAB Response to the Charge

The EAB thanks Sandia management for the opportunity to review this important project, and looks forward to advising the Born Qualified team throughout the three-year duration of the Grand Challenge (GC). Comments in response to the Charge are given below.

Strategy

Sandia has assembled an outstanding high-performance team to address an extraordinarily complex materials qualification problem over the long term. Both the 15-year vision and initial steps proposed for the three-year GC are bold and potentially transformative. The EAB reminded Sandia to keep the focus on the challenges of qualification and not on the additive manufacturing (AM) process, which remains but one of many methods to produce components that require qualification.

As discussed at length during the meeting and in the outbrief session, both the 15-year vision and the three-year project plan are in critical need of a roadmap that outlines where the overall effort is headed and where / how each aspect plugs in, so that every person working on the project knows what he / she is expected to contribute. The EAB does not wish to micro-manage the roadmap; it is clear that each project team is highly capable and understands the issues it faces. (In this connection, the EAB also commended Sandia for identifying an individual responsible for each task area.) Nonetheless, the overall team effort needs a template to execute against; some thoughts and suggestions follow.

The roadmap needs to begin with a thorough understanding of state of the art within each task area – what can be done today; what can realistically be accomplished within three years; what are the important milestone in the mid- to long-term. The team should determine the dependencies – what each task area requires from the others in order to accomplish its goals. Sandia should also consider the inclusion of insertion opportunities following the achievement of maturity stages in the evolving certification methodology or capability steps. These could include relevant directed stockpile work projects.

The EAB likes the use of exemplars to focus efforts within the GC and believes that each has been chosen carefully on the basis of sound criteria. Based on the needs of these exemplars, the team should conduct an analysis of the optimal approach for each – what materials, what methods, and what unique challenges must be overcome. Those determinations then lead to the design of experiments or deliverables required for each task area. (For example – a metal part can probably be printed now, whereas a ceramic exemplar will require much more time and fundamental research. The strong link / weak link exemplar may be more of a design optimization problem than a manufacturing one. Let each exemplar determine its own needs.)

Another important question to keep in mind as the roadmap is constructed is – what are the critical variables that need to be controlled? This helps the team determine the best approach to certain problems. If, for example, you don't have access to the most critical process parameter on a vendor's AM machine, then the better approach might be to dial back to a test bed where you can control that variable yourself. If you have to build your own machine rather than use

one from a vendor, that will require more project resources -- leaving less for other tasks. It is important to determine these priorities early on.

Finally, one EAB member pointed out that since it is Sandia's intent to "fundamentally change the engineering design and qualification paradigm" the BQ roadmap should demonstrate early on the baseline qualification processes and procedures that will be replaced with this new paradigm. Such an exercise is essential, admittedly difficult, and often left until too late in an ambitious program such as this one. This recommendation represents considerable work for the exemplar teams, but for the proposed interim EAB meeting in May / June, it would be helpful to see some definition of the existing qualification processes / procedures / validations for each. In essence, this provides a baseline for the roadmap requirements.

As noted in "Impact" below, the board believes that impact will result if qualification is defined. The baseline suggested above will be necessary to achieve impact and to understand its magnitude. While the qualification is of primary importance and thus should receive the most emphasis, the Charge given to the board includes "engineering design." This suggests that the roadmap should also include a baseline for how engineering design is currently achieved for the three exemplars, and illustrate a path to the anticipated process flow for the "new paradigm."

The EAB has the sense that the participants have plenty of experience in managing big projects and should be able to assemble such a roadmap in short order. We would like to discuss via conference call / webinar within roughly three months' time (e.g. by late May / early June).

Overall, the board believes that the BQ team is addressing the right issues and has the talent required to make real progress. The initial scope is necessarily broad but will be funneled down to the best set of activities within the first year as dictated by the roadmap. The EAB also urges the team to include specific interim "wins" that concretely demonstrate progress to the project's sponsors – don't try to wait and demonstrate a single big win at the end.

One risk identified by the EAB is overall data management. Both the models and the experiments will produce massive amounts of data, and it was not clear to the board how the team planned to gather, store, and process the data. In addition, "big data" techniques may be helpful in the analysis and may provide unexpected insights that are useful to modelers and experimentalists. The EAB recommends that a capable data scientist should be added to the team.

Relevance

The project clearly has direct relevance to the mission of its nuclear weapons sponsor, and Sandia has both unique needs and deep technical capabilities that it can bring to bear on materials assurance in advanced manufacturing. The EAB was impressed with both the foundational work that Sandia has performed over several decades, as well as numerous supporting activities (such as the work in Predicting Performance Margins, uncertainty quantification, verification, and validation, related LDRD projects, and topological optimization).

Both the difficulty of the problem and the scope of work that Sandia can pull together into a single multi-disciplinary effort make this a project worthy of a national laboratory. The EAB commends Sandia for "harnessing" its capabilities in microstructure-sensitive modeling and multiscale, multiphysics systems to address modeling of AM processes and resulting structure-property relations.

The board believes that Sandia's advantage is the scope and breadth of technology end-to-end that SNL can bring to bear on the problem through a talented multi-disciplinary team. The Lab's special strengths are judged to be in computational multiscale modeling of materials processing, microstructure-property relations, and structural mechanics, uncertainty quantification, and materials science.

Quality

While it is clear that Sandia approaches its work with a high degree of scientific integrity, it is too early for the EAB to offer meaningful comments. The specific technical goals are not yet clear enough and need to be laid out in the roadmap as described above. The EAB looks forward to discussing the roadmap in May and reviewing Sandia's work at the next meeting in October.

Topics where Sandia's capabilities appear to be leading edge are listed under Relevance above (modeling, uncertainty quantification, and fundamental materials science.)

Workforce / Capabilities

The researchers working on the project all appear to be high caliber, and the EAB was particularly impressed with the early career staff.

On the question of partnerships, the board emphasizes that this should be part of the initial research that goes into the roadmap – determine who is best at a particular task that Sandia needs to accomplish and establish partnerships as needed; don't be trapped into thinking you are the best at everything that is important. The modeling team seems to be well grounded in this approach; aware of current state of the art and working with those who have advanced models (LLNL's powder bed model, for example). The EAB also pointed out that aerospace companies face very similar problems in qualifying high-reliability components. All members emphasized that Sandia has "open access" to capabilities available at their institutions; visits to Oak Ridge and Lockheed Martin have already been arranged and more are forthcoming.

Impact

This project will have impact if it can determine what defines qualification and where it can be inserted into a manufacturing process. The problems Sandia seeks to solve are the toughest ones, and if BQ can be used to qualify a highly critical component such as a gas generator valve, the same principles can be applied almost anywhere. Satellites, bridges, ships -- the potential legacy is enormous.

Referring back to comments made in the "roadmapping" section of Strategy, a baseline is needed for processes / procedures / verifications for qualification and design if the team is to understand and measure the effects of the changes being proposed.

As noted earlier, the team should not forget to define easier targets along the roadmap. The ultimate BQ goal will take a long time to achieve, but much can be spun off as it is learned. It is also important to demonstrate interim wins to maintain the long-term support of sponsors. The pathway to future funding needs to be as clear as the technical roadmap – When we get to Year 4, who will be funding the effort? What do we have to show them to secure their support?

VI. Next Meeting

The EAB looks forward to the interim telecom in May, and to the next meeting on October 20 – 21, 2016.

VII. Session Agenda

Born Qualified Grand Challenge External Advisory Board Meeting

March 2-3 2016 | Building 960 / Room 1001 A & B Sandia National Laboratories | Albuquerque, NM

Wednesday, March 2, 2015

8:30–8:45 am	Welcome & Charge for the Day—Andy McIlroy
8:45–9:00	Sandia National Laboratories' LDRD Program—Andy McIlroy
9:00–9:15	Opening Remarks—Terry Aselage
9:15–10:00	Born Qualified Overview—Allen Roach
10:00-10:15	Break
10:15-11:00	Exemplars & Sandia Impact—Dorian Balch
11:00-11:30	Open Discussion
11:30-12:15 pm	Lunch
12:15-12:55	Properties *Al Instante,* Rapid High-Throughput Screening of Stochastic Properties—Brad Boyce & Harlan Brown-Shaklee
12:55-1:35	Optimization Ideas & Approaches—Bart van Bloemen Waanders
1:35-1:50	Break
1:50-2:40	Multi-scale, Multi-physics Models—Mike Chandross & Joe Bishop
2:40-4:00	Poster Session
4:00-4:45	EAB Executive Session
4:45-5:00	Questions from EAB/Discussion

Born Qualified Grand Challenge External Advisory Board Meeting

March 2-3 2016 | Building 960 / Room 1001 A & B Sandia National Laboratories | Albuquerque, NM

Thursday, March 3, 2015

8:30-8:45 am	Welcome, Review of Day One—Allen Roach/Melecita Archuleta
8:45 – 9:15	Overview of AM Process Plans—Bradley Jared and Chris Diantonio
9:15 – 9:45	Partner Presentation–PPM—Corbett Battaile
9:45-10:00	Wrap up & Discussion
10:00-11:00	EAB Executive Session (Closed)
11:00-12:00 pm	Lunch & EAB Out Brief—Craig Blue

APPENDIX B: EXTERNAL ADVISORY BOARD REPORT #2

External Advisory Board Report
Meeting: October 20-21, 2016

Born Qualified Grand Challenge LDRD

Sandia National Laboratories

This report is presented to Rob Leland, Vice President and Chief Technology Officer (CTO) and Andy McIlroy, Director of Research Strategy and Partnerships, and to the Born Qualified Grand Challenge LDRD project team at Sandia National Laboratories (SNL) by its External Advisory Board (EAB), following the meeting of October 20-21, 2016 in Albuquerque, New Mexico. This was the second meeting of the Born Qualified EAB, the first meeting was held on March 2-3, 2016.

7. I. SUMMARY FEEDBACK

The EAB commends the team for having worked very hard and accomplishing much in this initial "Year of Discovery." The progress made and the foundation laid as a result of this discovery phase should now lead to important accomplishments in Years 2 and 3.

The response from the BQ team has been thorough and impressive – both in terms of constructing the roadmap and defining the three-year goals of the Grand Challenge (GC) project within Sandia's 15-year vision. The team is now clearly focused on the issue of qualification. In our view, Sandia has assembled a complete plan to rewrite qualification that is globally unique – we are not aware of any other such effort that addresses this critical problem on such a comprehensive scale.

The team should now think carefully about what should happen starting in Year 4. If it is expected that a customer such as Sandia's Nuclear Weapons (NW) program will fund a continued effort, then what information and results will be needed in order to justify it? There must now be a clear and deliberate path to that accomplishment through Years 2 and 3.

To this end, the EAB recommends that the team should decide what are the one or two highest-priority outputs of the GC. The project plan and all individual contributions must then be focused on those few essential elements. A suggested set of decision matrices to help identify those elements is suggested in the body of the report below. We also encourage the BQ team to formulate the unique vision of the project more concretely and concisely in a succinct statement that can be communicated effectively throughout the NW community.

Because Sandia proposes to write the rules of qualification, it will be necessary to communicate the importance and utility of the proposed process and methods. BQ needs to develop an external communication plan, comprised of both a position paper at the end as well as publications along the way that establish credibility for that final product.

The EAB very much liked the single-slide optimization strategy and recommends that it should be adopted by the entire team. Given the complexity of this project, we believe that this kind of disciplined project management would be very helpful. This approach would also help all modelers and experimentalists to embrace data science as a priority. The board believes that data science can be the differentiator in this project; Sandia has both a great technical team and the right culture in Verification / Validation / Uncertainty Quantification (VVUQ) to achieve real success here.

The board noted that the BQ team is pursuing a lot of different models at different length scales, and understand these are necessary given the objectives of the project. Nonetheless, there should be a concerted effort to reduce redundancy between models wherever possible.

Sandia needs to remain closely attuned to the needs of the external community. The EAB raised a concern that Sandia is working with two metal AM machines, one of which is outdated and the other which is unique to SNL. What will be important over the long term is that Sandia's qualification methodology will be machine agnostic and can be applied as manufacturers continue to improve their equipment. The board also emphasized the importance of the relationship between witness objects and build objects – this is an extremely difficult problem, but one that is central to the whole issue of qualification.

The EAB requested that the BQ team should discuss the results of its decision matrix exercise, as well as its draft communication plan, in a telecon meeting by the end of January 2017. Our next regularly scheduled meeting will take place around July 2017.

Summary comments with respect to Sandia's five assessment elements are given below:

Strategy: The EAB believes that the BQ team is pursuing goals that are both bold and transformative. Sandia's effort is globally unique; for this reason, we place great emphasis on the need for outreach.

Relevance: As discussed at the first EAB meeting, the project demonstrates clear relevance to Sandia's nuclear weapons mission.

Quality: To the question "Is the research demonstrated to date of high quality and at the leading edge?" the board responds: Absolutely. We were especially impressed with what we saw in analysis, modeling, and UQ.

Capabilities: The work presented by Sandia's early career staff, especially in the poster session, was highly impressive. Their enthusiasm is infectious, and we enjoyed interacting with them. Please continue to keep a slot in the agenda for a poster session – we find it very informative.

Impact: The bulk of our comments in this report pertain to impact. It appears to us that the BQ team is focused on the issue of qualification and has assembled all the necessary pieces, but we cannot yet state clearly whether Sandia is on the path to achieve high impact. The goal must be to attain impact for Sandia's NW program and for the outside world. The BQ team needs a succinct statement of the goal that embodies the intended impact and that can be communicated quickly and effectively throughout the NW community.

II. Board Members

Members Present

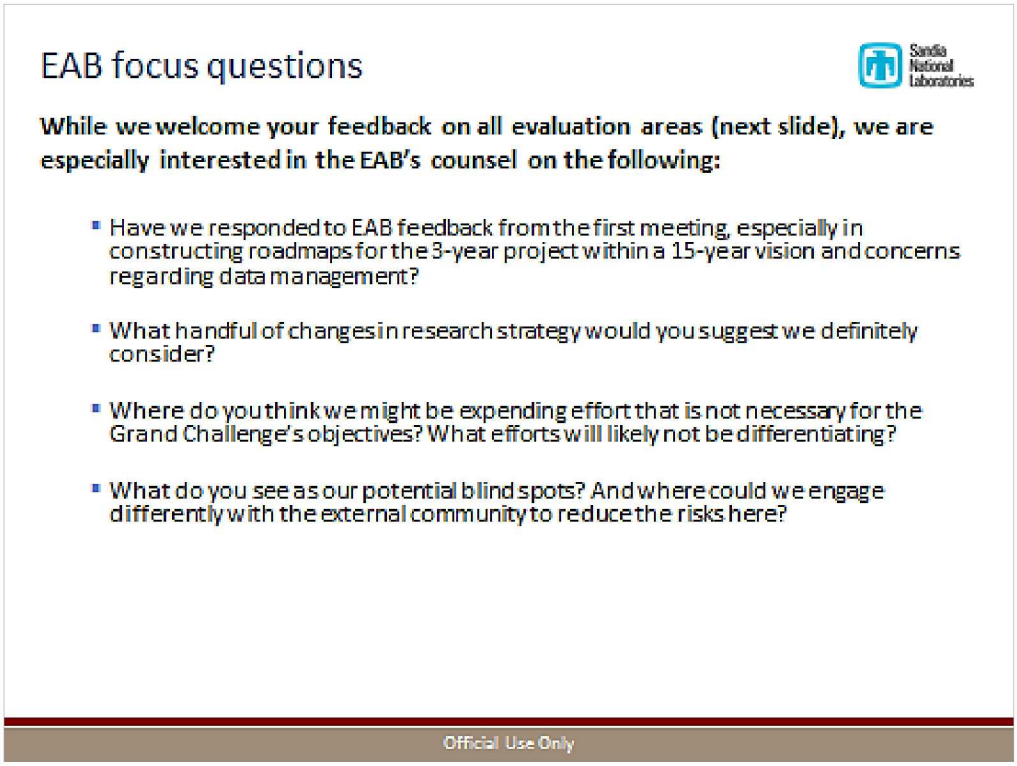
- **Slade Gardner**, Acting EAB Chair, President, SG Advanced Manufacturing and Materials
- **Elizabeth Holm**, Professor of Computational Materials Science, Carnegie Mellon University
- **Daryl Landeg**, Chief Technologist, Atomic Weapons Establishment (AWE), UK
- **David L. McDowell**, Executive Director of the Institute for Materials, Regents' Professor and Carter N. Paden, Jr. Distinguished Chair in Metals Processing, Georgia Institute of Technology

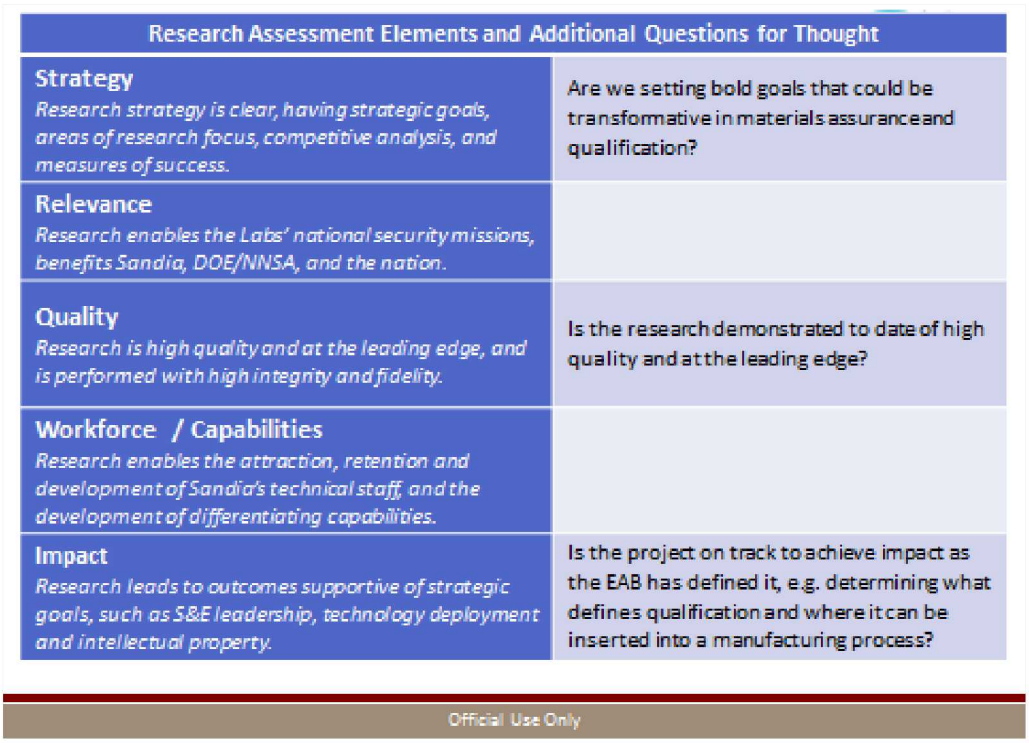
Members Absent

- **Craig Blue**, EAB Chair, Chief Executive Officer, The Institute for Advanced Composites Manufacturing Innovation (IACMI); Director of the Advanced Manufacturing Office and the Manufacturing Demonstration Facility, Oak Ridge National Laboratory
- **David McMindes**, Chief Technology Officer, National Securities Campus, Honeywell Federal Manufacturing & Technologies, LLC. (FM&T)
- **William Tredway**, Leader, Advanced Manufacturing Technology, United Technologies Research Center

III. Charge to the EAB

The Board was provided with a set of questions to guide its evaluation of the project as presented. These are given below.





Research Assessment Elements and Additional Questions for Thought	
Strategy *Research strategy is clear, having strategic goals, areas of research focus, competitive analysis, and measures of success.*	Are we setting bold goals that could be transformative in materials assurance and qualification?
Relevance *Research enables the Labs' national security missions, benefits Sandia, DOE/NNSA, and the nation.*	
Quality *Research is high quality and at the leading edge, and is performed with high integrity and fidelity.*	Is the research demonstrated to date of high quality and at the leading edge?
Workforce / Capabilities *Research enables the attraction, retention and development of Sandia's technical staff, and the development of differentiating capabilities.*	
Impact *Research leads to outcomes supportive of strategic goals, such as S&E leadership, technology deployment and intellectual property.*	Is the project on track to achieve impact as the EAB has defined it, e.g. determining what defines qualification and where it can be inserted into a manufacturing process?

IV. Meeting Logistics

The EAB review session was held on Thursday and Friday, October 20-21, 2016 in Albuquerque, NM. On Thursday, Greg Frye-Mason, LDRD Program Manager, welcomed Sandia's guests and presented the Charge to the EAB. Kate Helean, Program Manager (PM), provided opening remarks and an overview of additive manufacturing at Sandia. Allen Roach, Principal Investigator (PI), then gave an overview on the Born Qualified (BQ) project, technical progress since the last meeting, and a review of the roadmap developed by the BQ team subsequent to the first EAB meeting.

These overviews were then followed by a series of detailed technical presentations from BQGC team leads. The day concluded with a poster session and a closed EAB session, during which the members discussed their impressions of material presented throughout the first day.

In the second half-day session on Friday October 21, the EAB heard additional technical presentations and conducted a final executive session. The board then presented its preliminary findings in an outbrief to SNL management and the BQGC team. The meeting concluded following questions and discussion by the whole group.

An agenda detailing talk and poster titles and presenters is attached at the conclusion of this report.

V. EAB Response to the Charge

The EAB appreciates the opportunity to provide this second review of the Born Qualified (BQ) Grand Challenge at Sandia and commends the team for having worked very hard and accomplishing so much in its first year. This has been the "Year of Discovery," characterized by problem identification and team formation. The progress made and the foundation laid as a result of this discovery phase should now lead to important accomplishments in Years 2 and 3.

Have we responded to EAB feedback?

The response from the BQ team has been thorough and impressive – especially in constructing the roadmap around the project's three exemplars, through which a common set of science challenges are addressed. In addition, the team is now clearly focused on the issue of qualification. In our view, Sandia has assembled a complete plan to rewrite qualification that is globally unique – we are not aware of any other such effort that addresses this critical problem on such a comprehensive scale.

The team also responded to the EAB's request to more clearly define the three-year goals of this Grand Challenge project within Sandia's total 15-year vision. We suggest that the team should now think carefully about what should happen starting in Year 4 after this initial project has concluded. If it is expected that a customer such as Sandia's Nuclear Weapons (NW) program will fund a continued effort, then what information and results will be needed in order to justify it, and what is the work package that will produce those desired results? There must now be a clear and deliberate path to that accomplishment through Years 2 and 3.

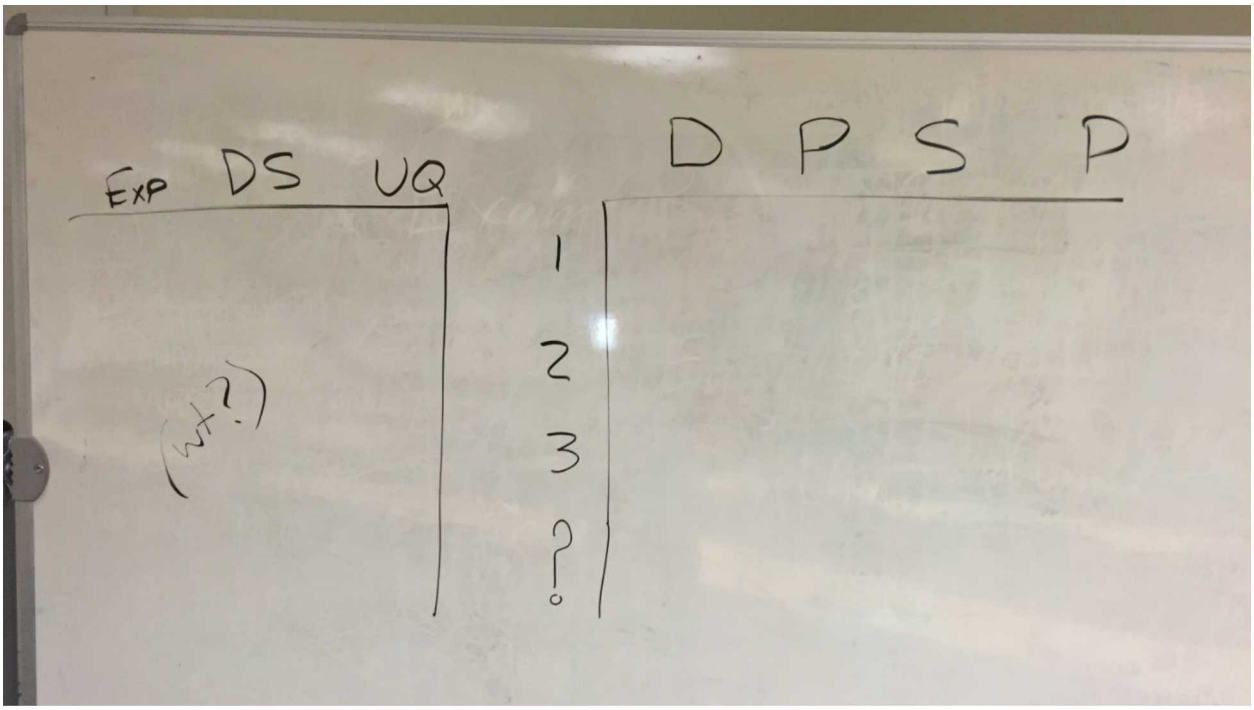
To this end, the EAB recommends that the team should decide what are the one or two outputs of the GC effort that are of highest priority, and what else then becomes "nice to have" or non-essential to the most important goals. The project plan, resources, and every team member's contributions to the effort must then be focused on those few essential elements. If there are means by which elements such as high throughput testing could be funded by other efforts, thus allowing core funds to support other core efforts in modeling and experiments, this should be undertaken. We also encourage you to formulate the unique vision of this project more concretely and concisely to facilitate quick and ready communication of the program impact to executives without a background in the specific technologies of BQ. (One starting point might be to better illustrate the overall cost story; for example, the ability of BQ to reduce the cost / schedule from $$ / years to $500K / 3 months.)

Because Sandia proposes to rewrite the rules of qualification, it will be necessary to communicate to the world the importance and utility of the proposed process and methods. Thus, we recommend that BQ needs to develop an external communication plan. This would comprise both a position paper or thought piece at the end (such as a white paper delivered to relevant communities like NRC, NIST, DOE and DoD), as well as publications, conference presentations, etc., along the way that set the stage and establish credibility for that final product. We would like to see this plan and discuss it with the team within three-month's time from the conclusion of this meeting.

The EAB very much liked the single-slide optimization strategy presented at the Friday morning session and recommends that it should be adopted by the entire team. This would allow BQ to reflect all tasking, players and handoffs in a single plan, so that each contributor knows exactly where and when they fit in the strategy. Given the complexity of this project, we believe that this kind of disciplined project management would be very helpful.

What handful of changes in research strategy should we consider?

As discussed at the outbrief, the EAB suggests that the BQ team should construct and examine two decision matrices (see whiteboard snapshot below). The first is to take the DPSP (Design-Process-Structure-Properties) matrix and rank each of the exemplars in terms of impact on each of these priorities. This identifies what each exemplar can be expected to deliver for the three-year program. While one exemplar may have strong impact against all priorities, another exemplar may only have applicability to one or two of these priorities. This will set team expectations for the depth and breadth of investigation on the exemplars. The second matrix uses weighting factors determined by the PM and PI to rank each exemplar for the potential quality of experimental data, data science and uncertainty quantification achievable within the context of the three-year program. This will provide an understanding of what aggregate value can be extracted from a given exemplar, thus how much of the project's limited resources should be applied. The goal is not necessarily to eliminate any of the exemplars, unless that becomes clear in this process, but rather to understand where the value for each resides and how much of the program resources are appropriate to extract that value.



The EAB would like to hear the outcome of these analyses and the resulting plan within the next three months (i.e., by the end of January 2017).

Where might we be expending effort that is not necessary?

The EAB noted that the BQ team is pursuing a lot of different models at different length scales, and understands these are necessary given the objectives of the project. Nonetheless, there should be a concerted effort to reduce redundancy between models wherever possible – for example, there appear to be multiple melt pool models in play. We recommend that the team

should examine all the models in a workshop to make sure that everyone is using the same understanding, inputs, boundary conditions, and evaluation criteria. This would assist in sorting out best practices and enhancing the value delivered for the investment made.
The board would like to see more data science injected into the analysis; at present, it still appears to be an "island" within the larger effort. This is a key element of the optimization strategy presented to us, and the need for all modelers and experimentalists to embrace data science as a priority represents a cultural challenge that Sandia is well equipped to meet. We also urge that data scientists should be active participants in the experiments and that experimental data be made available for analysis immediately. The board believes that data science can be the differentiator in this project; Sandia has both a great technical team and the right culture in VVUQ to achieve real success here.

What are our potential blind spots?

Sandia needs to remain closely attuned to the needs of the external community. An example cited during discussion is Doug Wells' upcoming NASA Marshall report* that spells out NASA's view of Inconel 718 structures produced by powder bed fusion. Much of this report will not be applicable to Sandia's work, but it does represent a two-year effort that has been vetted throughout the industrial and research communities. The team should therefore study it and extract whatever feedback might be useful to the BQ strategy, then modify its findings in accordance with Sandia's experimental results.

As noted earlier, the team should keep in mind what is important to its future sponsor and keep the work focused there – we caution against getting too caught up in what might be "cool science" but is unlikely to advance the most important objectives.

The example of the silicone foam pad that arose during discussion is an important opportunity – there is real customer adoption potential, and a good bit of data, processing, and test experience already exists. This may not be a formal exemplar case study; however, BQ should have some level of case study for the silicon foam pad. This is important from both a customer relationship perspective as well as that of a success point. Anything that can be learned about the DPSP for the silicone foam pad and studied with data science and uncertainty quantification should be regarded as a valuable opportunity to show the power of BQ. It would be valuable to include the silicone pad as an opportunity against the exemplars in the decision matrices described above.

The EAB also raised a concern with respect to metal AM – Sandia has two machines on site; one of which is outdated and the other unique to SNL. We understand that the LENS system is great for data collection, but it is not used widely by others. For this reason, we believe that the best use of LENS under the BQ umbrella is to diagnose a qualification method, not to develop new materials and AM processes. What will be important over the long term is that Sandia's qualification methodology will be machine agnostic and can be applied as manufacturers continue to improve their equipment. A plan to apply BQ methodology to other machines may

* "**Overview of Fatigue and Damage Tolerance Performance of Powder Bed Fusion Alloy N07718**," Douglas Wells, NASA Marshall Space Flight Center, presentation at ASTM Committee E08 / NIST Workshop on Mechanical Behavior of Additive Manufactured Components; May 4, 2016; San Antonio, TX [access presentation here and Wells' book with the same title here]

be examined with external relationships or contract builds on other machines. Perhaps this is a Year 3 test of the BQ methodology.

One key point to keep in mind is the relationship between witness objects and build objects – are you actually testing something that gives insight into the build object? The board realizes that this is an extremely difficult problem, but one that is central to the whole issue of qualification. Regarding collaborators, Sandia seems to be well aware of other efforts underway within DoD (Navy and AFRL) and at LLNL. If efforts in glass printing continue following completion of the matrix analysis, then collaboration with MIT might be worthwhile.

Other Comments

The board was intrigued by the whole emerging issue of stockpile responsiveness. While this is not something that Sandia can influence, it is worth thinking about the implications and being prepared to respond if BQ can address such emerging needs.

In conducting the matrix assessment outlined above, the BQ team should not just focus on the Technology Readiness Level (TRL) of the exemplars – a certain level of Manufacturing Readiness Level (MRL) is probably required as well. Think about MRL hurdles that may need to be overcome as you assess the maturity of the technologies under consideration.

One final thought: Given the timescale for the overall vision (15 years) and the rapid pace of development, it may be worth considering the potential of machine learning in the context of BQ.

VI. Next Meeting

The target date for EAB #3 is around July 2017. The exact date should be fixed as soon as possible, as members of the board who serve in academia are often traveling at that time, and calendars are already filling up for all participants. It would also be appreciated if the meeting could end earlier than on Friday afternoon, allowing our long distance travelers a better opportunity to get home for the weekend.

VII. Session Agenda

Born Qualified Grand Challenge External Advisory Board Meeting

October 20-21 2016 | Building CSRI / Room 90

Sandia National Laboratories | Albuquerque, NM

Thursday October 20, 2016

8:00–8:15am	Welcome & Charge for the Day—Greg Frye Mason
8:15–9:00	Opening Remarks and AM Overview—Kate Helean
9:00–9:45	Born Qualified Overview, Updates, Roadmap—Allen Roach
9:45-10:00	Break
10:00-10:45	Ceramic Exemplar Status—Dan Kammler
10:45-11:30	GTS Exemplar—Dorian Balch
11:30-12:15pm	Lunch
12:15-12:45	Failsafe Exemplar—Nick Leathe
12:45-1:30	Alinstante—Kris Klingler
1:30-2:00	Multiple Scale Powder Bed Fusion Models—Mario Martinez
2:00-2:30	Process–Structure–Performance of Metal Additive—Joe Bishop
2:30-3:30	Poster Session with One Minute Introductions
3:30-5:00	EAB Executive Session / Questions / Discussion

Friday October 21

8:00-8:15am	Welcome, Review of Day One—Allen Roach/Kate Helean
8:15-8:45	Ceramic and Glass Models—Kurtis Ford
8:45-9:30	Optimization & Data Science–Bart van Bloemen Waanders & Laura Swiler
9:30-10:00	Wrap up & Discussion
10:00-11:00	EAB Executive Session (Closed)

11:00-12:00 pm Lunch & EAB Out Brief—Slade Gardner

VIII. Poster Session

Born Qualified Grand Challenge External Advisory Board Meeting

October 20-21 2016 | Building CSRI / Room 90

Sandia National Laboratories | Albuquerque, NM

Poster Session

1. Administrative: Roadmap, Publications, Deliverables—Allen Roach
2. Collaborations — Sita Mani
3. Thermal-Structural Modeling of LENS AM — Kyle Johnson
4. Texture Process Models for Metal AM — Judith Brown
5. Towards In-Process Materials Characterization in Laser-Based Metal Additive Manufacturing — Nic Argibay and Andrew Kustas
6. Correlating Defect Populations with Mechanical Performance in AM Tensile Samples of PH 17-4 — Olivia Underwood
7. AM Coupon for Nondestructive Material Characterization — Nick Leathe
8. Compositional Analysis for Additive Manufacturing — Mike Brumbach

APPENDIX C: EXTERNAL ADVISORY BOARD REPORT #3

External Advisory Board Report
Meeting: July 19 - 20, 2017

Born Qualified Grand Challenge LDRD

Sandia National Laboratories

This report is presented to Susan Seestrom (Chief Research Officer) and Grant Heffelfinger (Director, Advanced Sciences & Technology Program Management) and to the Born Qualified (BQ) Grand Challenge project team at Sandia National Laboratories (SNL) by its External Advisory Board (EAB), following the meeting of July 19 - 20, 2017 in Albuquerque, New Mexico. This was the third meeting of the Born Qualified EAB.

I. Summary Feedback

The EAB thanks Sandia for the opportunity to continue its assessment of the Born Qualified LDRD Grand Challenge and is impressed with both the scope of the project and with the team's refreshingly honest assessment of what it believes can be achieved with the available budget. For reasons outlined in the report that follows, the board recognizes that the BQGC is truly at the cutting edge of technology. The modeling work is outstanding, especially the thermal and structural modeling of the additive manufacturing (AM) process and its demonstrated ability to provide downstream prediction. The board further commends the team's strategic planning efforts, and the manner in which the BQ message is being communicated across the Lab.

Sandia is building an outstanding modeling and prediction infrastructure and is making solid progress on an elegant risk-averse optimization scheme, but lacks the high quality, reproducible data to validate that infrastructure, and the optimization scheme may not be mature enough to apply to the exemplars in Year 3 of the project. The board is also concerned that the effort to correlate microstructure of the high-throughput dog-bone coupons appears to require a breakthrough – which is notoriously difficult to achieve, especially on a schedule. The BQ team needs to perform a risk analysis against execution of the strategic plan and develop a firm schedule for the remainder of the project. The first set of exemplar builds should also be started as early as possible. If a breakthrough is essential to success, then efforts should focus strongly on making it happen, along with a clear "Plan B" in case it cannot be achieved by a given Go / No-Go point. The EAB would like to hear the mitigation plan by mid-September.

The use of models, *in-situ* process data and rapid test / characterization methods to create probabilistic predictions that identify quantitative qualification thresholds is unique to the BQ Grand Challenge. This lies at the heart of Sandia's goal to fundamentally change the qualification process. If successful, this will have immediate impact on the nation's weapons complex and eventually across the field of advanced manufacturing. The goal is an important one; worth "naming and claiming" – we encourage the team to think of a name to brand it.

The EAB affirms that the BQ team has done a good job of crisply articulating the goals of the three-year project; we will comment on whether they are track to achieve those goals after reviewing the risk mitigation plan and revised schedule at the September telecon.

The Born Qualified work is clearly on part with leading-edge efforts; an exact assessment is difficult to make because there are few examples at this scale and

caliber that can be reasonably compared. Sandia needs to be doing more in terms of outreach; both in terms of making the community aware of its work and in obtaining critical data now to populate its modeling infrastructure. The EAB believes that the project is on track to produce the appropriate number of publications, patents, and technical advances.

Due to the nature of the challenges summarized throughout this report, the EAB recommends that the program be fully funded in the final year, or if possible, additional financial resources should be made available. Any funding reductions will severely jeopardize the ability of the BQ team to meet its objectives in the final year.

II. Board Members

Members Present

- **Slade Gardner**, Acting EAB Chair, President, SG Advanced Manufacturing and Materials LLC
- **David L. McDowell**, Executive Director, Institute for Materials, Georgia Institute of Technology
- **David McMindes**, Chief Technology Officer, National Securities Campus, Honeywell Federal Manufacturing & Technologies, LLC. (FM&T)
- **William Tredway**, Leader, Advanced Manufacturing Technology, United Technologies Research Center

Members Absent

- **Craig Blue**, Director, Energy Efficiency and Renewable Energy Programs, Oak Ridge National Laboratory
- **Elizabeth Holm**, Professor of Computational Materials Science, Carnegie Mellon University
- **Daryl Landeg**, Chief Technologist, Atomic Weapons Establishment (AWE), UK

III. Charge to the EAB

The Board was provided with a set of questions to guide its evaluation of the project as presented. These are given below.

EAB focus questions

While we welcome your feedback on all aspects of the Born Qualified LDRD Grand Challenge project, we are especially interested in the EAB's counsel on the following:

Whereas Year 1 of the project was devoted to Discovery and the current Year 2 to developing the necessary Capabilities in modeling, measurement, and data management, in Year 3 we will measure predicted performance against the actual manufacture of exemplar parts.

- What do you regard as the most significant accomplishments along this path to date?
- What do you foresee as the biggest challenges in Year 3, and what else do we need to be doing to prepare for them?
- Based on progress to date and the current project plan, what portions of the effort seem most likely to be highly differentiating for Sandia?

3

EAB focus questions

- At the last EAB meeting, the board felt it was too early to judge whether Born Qualified was on the path to achieve high impact, and also recommended that the team needed a succinct statement of the goal that embodies the intended impact.
  - Have we presented a succinct statement of the goals, and are we now on track to achieve these goals? Why or why not?
- In your estimation, is the quality / potential impact of the work on par with leading work in the field? Where is it stronger, and where is it weaker?
- Is the work being sufficiently documented / shared with the community? (Publication plan)

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IV. Meeting Logistics

The EAB review session was held on Wednesday and Thursday, July 19 - 20, 2017 in Albuquerque, NM. On Wednesday, Greg Frye-Mason, Laboratory Directed Research and Development (LDRD) Program Manager, welcomed Sandia's guests and presented the Charge to the EAB. Kate Helean, Project Manager, provided opening remarks along with an overview of additive manufacturing at Sandia, followed by an overview and update on the project from Allen Roach, Principal Investigator.

These introductory presentations were followed by a series of detailed technical talks on the project's modeling efforts. Following lunch, the BQ Leadership and the board members attended tours highlighting the project's experimental efforts, followed by a poster session and a closed EAB executive session.

Thursday's half-day session began with technical presentations on the project's efforts in data science and optimization, along with general discussion. The board then conducted a final executive session and presented its preliminary findings in an outbrief to SNL management and the BQGC team. The meeting concluded following questions and discussion by the whole group.

An agenda detailing talk titles and presenters is attached at the conclusion of this report.

V. EAB Response to the Charge

The EAB thanks Sandia for the opportunity to continue its assessment of the Born Qualified LDRD Grand Challenge and is impressed with both the scope of the project and with the team's refreshingly honest assessment of what it believes can be achieved with the available budget. The board recognizes that the BQGC is truly at the cutting edge of technology, challenging the available materials, equipment and depth of knowledge to achieve a meaningful paradigm shift that accelerates optimization and qualification. The mission is admirable, the skill and talent are unmatched and the execution / adjustments to date have been excellent. The board is pleased to note that the team has responded so positively to the advice provided at the two prior meetings and hopes that the advice offered during discussions and in this report, will be helpful as well.

Most Significant Accomplishments

The modeling work is outstanding, especially the thermal and structural modeling of the AM process and its demonstrated ability to provide downstream prediction. SNL should make every effort to protect the mesoscale modeling Intellectual Property (IP) and make it available to other outlets through licensing or other appropriate means. If additional budget can be found, then the mesoscale modelling work could be applied to materials, machines and processes beyond the scope of the exemplars to leverage this IP against a wide range of license opportunities.

The board also commends the BQ team's strategic planning efforts, which have matured greatly since the first meeting – every individual we spoke with had a clear idea of how his / her effort fits into the roadmap that the team has developed. It was also clear that the BQ effort reaches out into many programs across the entire Laboratory; it seems that virtually every individual team member is also involved in important mission work and is communicating the BQ message across the Lab. It would be worthwhile to document these interactions, as they clearly show that Born Qualified is producing important benefits to the programs and can be expected to continue to provide benefit beyond the conclusion of a three-year LDRD project.

The high-throughput testing approach is novel in that large amounts of data can be quickly generated and the Digital Image Correlation data is powerful for structure-process-property relationships. This capability is a powerful tool and the board recognizes the impact that it could have, however the test data available thus far for dog-bone coupons does not match the sophistication or quality of the method. Most of the effort has been devoted to creating the structure-property relations, yet the capability to include a focus on process parameters would provide a significant accomplishment. However, the board had difficulty understanding the full benefit of the *Alinstante* robot work in terms of necessity to efficient testing and procedure bottlenecks. Some automated tests are short duration and others are long duration, thus the process flow may not justify an integrated automated system. In the current form, it would seem to have greater impact in the outside world than "inside the fence" –

perhaps assisting, for example, a small company mapping out large data sets for various metals and alloys. As it is, companies are holding onto their own proprietary data and common, agreed-upon material standards are not emerging. In the right hands, Sandia's *Alinstante* approach could help accelerate that process.

Greatest Challenges in Year 3

Sandia is building an outstanding modeling and prediction infrastructure and is making solid progress on an elegant risk averse optimization scheme, but lacks the high quality, reproducible data to validate that infrastructure, and the optimization scheme may not be mature enough to apply to the exemplars in Year 3 of the project. Time is short, and much remains to be done.

If the new Renishaw machines are going to be used to produce the valve housing exemplar, the team needs to be validating the models and prediction infrastructure data with Renishaw machines now – yet those machines will not be installed until October or later, and it will take some time to get them running properly. It makes sense to be analyzing data now from other Renishaw machines – for example, those in use at the Kansas City plant or from another partner who could make the information available to Sandia. Another alternative might be to furnish a build file to Renishaw and have them supply test samples and process data.

The board is also concerned that the effort to correlate microstructure of the high throughput dog-bone coupons appears to require a breakthrough – which is notoriously difficult to achieve, especially on a schedule. The dog-bone test needs to be shown to have value with consistent results and material properties that correlate reasonably to materials science phenomenology before adopting it as practice. Rather than trying to correlate the strength and understand the variation, it would be more meaningful to show that consistent modulus is achievable first, then study the strength behavior. The breakthrough may be in using a better machine, such as the Renishaw, or in using a higher quality feedstock or better tuning of the process parameters (hopefully achievable with the Renishaw). If that breakthrough cannot be achieved, then the best alternative might be to focus on correlating process parameters to performance on the Renishaw machine that will be used to produce the valve housing exemplar.

The BQ team needs to perform a risk analysis against execution of the strategic plan and develop a firm schedule for the remainder of the project. The strategic plan flow chart should be evaluated block by block with an assessment of "what happens if this step does not succeed?". A contingency should be ready for each block. The board also recommends starting the first set of exemplar builds as early as possible. If a breakthrough is essential to success, then efforts should focus strongly on making it happen ("all hands on deck"). As part of this analysis, the team may need to consider whether to focus on a single exemplar rather than two or three as currently planned. If the risk is great that a required critical path cannot be achieved, then the alternative ("Plan B") needs to be defined, along with the criteria and timing that would trigger the switch to Plan B. The EAB would like to hear the team's risk assessment, schedule,

and mitigation plan by mid-September, before it launches into the third and final fiscal year of the project.

What Aspects are Highly Differentiating for Sandia?

Applying uncertainty quantification to performance predictions for the purpose of product qualification is highly differentiating. The use of models, *in-situ* process data and rapid test / characterization methods to create probabilistic predictions that identify quantitative qualification thresholds is unique to the BQ Grand Challenge. This lies at the heart of Sandia's goal to fundamentally change the qualification process. By combining this with optimization methodology it becomes more powerful yet, especially with the application of inverse optimization. As discussed during the meeting, Sandia is approaching this problem from first principles, whereas the rest of the world takes an empirical approach (determining what appears to be "good enough" and then locking it down with coarse safety factors that compensate for variance in data without concern for the cause of uncertainty). By contrast, Sandia's method attempts to quantify the material, process and characterization test control bands and employ s*tatistics* to predict performance. It also offers much higher fidelity in performance prediction, thus resulting in higher engineering design performance. If successful, Sandia's qualification will have immediate impact on the nation's weapons complex and eventually across the field of advanced manufacturing.

As discussed at previous meetings, Sandia's ability to incorporate Uncertainty Quantification into the optimization process is unique among peers. The EAB also feels that the highly calibrated IR camera demonstrated during the tours is differentiating for Sandia.

Statement of Goals

The EAB affirms that the BQ team has done a good job of crisply articulating the goals of the three-year project, both in the statements presented in the telecon following the second meeting and in the overview provided at this meeting. The cost saving estimate of 25%+ is likely extremely conservative, and more could be done to quantify the benefit of time savings, although this is admittedly difficult given large variations among materials, applications, etc.

It will not be possible to state whether the team is on track to achieve the goals laid out for the three-year project until the risk analysis and revised project plan have been presented. The EAB looks forward to evaluating these efforts in a September telecon.

At the outbrief, discussion arose as to whether materials or parts can ultimately ever be "Born Qualified," and if in fact this phrase may do more harm than good among a weapons community that regards such a concept as virtually impossible. The most useful understanding of the term is that it serves as a "North Star," a guiding principle that continuously provides direction, even if its ultimate achievement remains elusive. A

more realistic expression of the BQ goal might be that it provides a new way of probabilistic prediction that accelerates qualification.

It was also noted that, given the "Moore's Law"-like pace of innovation – especially in industry – that the overall BQ effort needs to be greatly accelerated, otherwise it will be left behind. The 15-year timetable probably needs to be reduced to roughly seven to eight years.

Comparison to Other Leading-Edge Work

The Born Qualified work is clearly on par with leading-edge efforts; an exact assessment is difficult to make because there are few examples at this scale and caliber that can be reasonably compared. Sandia is clearly leading the field in modeling, simulation, and uncertainty analysis. The most comparable example is probably NASA Marshall, who has taken on qualification and extensive analysis of a single alloy and is not diving so deeply into modeling and simulation. Nonetheless, what NASA has done well is to communicate its effort extensively to peer organizations and solicit their feedback. Sandia's effort seems insular and self-referencing by comparison. (In this connection, the board noted that Sandia's presentations could more clearly compare / contrast and recognize the work of others.) The EAB believes it would be worthwhile for Sandia to undertake outreach similar to NASA's, even if it extends only to the same organizations they approached.

Another form of outreach that Sandia might consider is hosting a workshop for industry. The goal would be to familiarize them with the BQ work and gain their insights, but the "data transfer" is likely to be one-way (transmit only) since industry will probably be reluctant to share data in an open setting. Nonetheless, such a workshop would be very valuable for the AM community as a means of starting dialog and could be supplemented with one-on-one meetings to share proprietary data with willing participants.

As noted earlier, Sandia's greatest need for outreach and assistance is in data generation – find the right partners to gain the high quality, reproducible Renishaw coupons and process data that BQ analysts need to exercise and validate the models and approach in preparation for producing the exemplars.

Publication Plan

Given the nature of this work, patents and technical advances are just as important to success as publications. That said, the EAB believes that the project is on track to produce the appropriate number of publications. The first publications are the hardest ones to get out, and it can easily take 18 months to get properly set up and produce publishable results. The board expects a "hockey stick" effect in the third year, with the most significant publications resulting during that time. It is worth pointing out that most of the posters already represent publishable work. The team should also be aware that

in order to get the work out by the end of year 3, the big push must come during the first half of the year – otherwise, the effort can come too late, and the work fails to get published. The EAB expects Sandia's work to be well received – "thank goodness somebody has been doing this!"

Other comments / advice:

There does not seem to be a good, simple two-word description that captures the scope of Sandia's BQ method. It might be worthwhile for the BQ team to create the nomenclature that labels this method. It would be good technical branding especially with the many publications ahead. Just to provide starting suggestions -- perhaps it is the 'S-P-P Probabilistic" method, or the "Statistical Phenomenology" method. These may not be appropriate but may illustrate possibilities that the team can improve on. We welcome a discussion at the September telecon.

Due to the nature of the challenges summarized previously, the EAB recommends that the program be fully funded in the final year, or if possible, additional financial resources should be made available. Any funding reductions will severely jeopardize the ability of the BQ team to meet its objectives in the final year.

VI. Next Meeting

The fourth EAB meeting should take place immediately after the first attempt at producing exemplars, with the goal of understanding lessons learned prior to undertaking the next round. According to the current plan, this would take place in May 2018 – but may change according to what the team presents in its risk / schedule analysis in September. Please suggest a date in connection with proposed schedule revisions when we conduct the telecon.

It was also mentioned that it might be interesting for the board to see the work being performed at the Advanced Materials Lab (located further away, at the UNM campus). We leave this to the discretion of the team.

VII. Session Agenda

Born Qualified Grand Challenge
External Advisory Board Meeting
July 19-20, 2017 | Building 822 / Room A & B
Sandia National Laboratories | Albuquerque, NM

Wednesday, July 19

8:00-8:15 AM	Welcome & Charge for the Day—Greg Frye Mason
8:15-9:00	Opening Remarks and Sandia AM Overview—Kate Helean
9:00-9:45	Born Qualified Overview & Updates—Allen Roach
9:45-10:00	Break
10:00-10:45	Thermal and Structural Modeling of the Metal Additive Manufacturing Process—Kyle Johnson
10:45-11:30	Ceramics Materials Models—Fadi Abdeljawad
11:30-12:15 PM	Lunch / LENS Process Model—Brad Trembacki
12:15-2:45	Tours • Tour 1 – 827 Test Bed (Murphy) • Tour 2 – 895 Alinstante (Klingler, Burchard) • Tour 3 – 701 Testing (Boyce) • Tour 4 – 878 AM (Jaren, Keicher, Cook, Mani)
2:45-3:45	Poster Session with One Minute Introductions
3:45-5:00	EAB Executive Session / Questions / Discussion

Thursday, July 20

8:30-8:30 AM	Welcome, Review of Day One—Allen Roach/Kate Helean
8:30-9:00	Progress & Challenges in Data Science—Laura Swiler
9:00-9:30	Integration—Bart van Bloemen Waanders
9:30-10:00	Wrap up & Discussion
10:00-11:00	EAB Caucus (Closed)
11:00-12:00 PM	Lunch & EAB Out Brief—Slade Gardner / Craig Blue, EAB

Born Qualified Grand Challenge
External Advisory Board Meeting
July 19-20, 2017 | Building 822 / Room A & B
Sandia National Laboratories | Albuquerque, NM

Poster Session

1. Nick Argibay and Andrew Kustas—Beyond 6.X Identifying an Improved Life Cycle for American Nuclear Weapons
2. Amber Dressler—Mechanical Property Variation in Metal Lattice Structures
3 Stepher Baier—MS&T Senior Design Group Project
4 Andrew Kustas—In situ and ex situ characterization of AM parts
5 Mark Wilson—Atomistic details of metal additive manufacturing in powder beds
6 Judy Brown—Modeling Microstructure Evolution and the Effects of Texture on Mechanical Properties in Additively Manufactured Metals
7 Samantha Taylor—Thermal History Correlation with Mechanical Properties for Polymer Selective Laser Sintering
8 Thao Nguyen and Jeremiah Sears—Large-scale, Low Temperature Cu Nanoparticle Syntheses for AM N-inks
9. Devonte Woodard and LaRico Treadwell—Next Generation of Materials (Low Z metals) for Digital Processing
10. Maddison Casillas and Francesca Fasulo—Synthesis of Alumina Nanoparticles for NInks

APPENDIX D: EXTERNAL ADVISORY BOARD REPORT #4

Sandia National Laboratories
Born Qualified Laboratory Directed Research & Development
Grand Challenge Project

External Advisory Board Review Meeting Report
Meeting Date: April 10-11, 2018

Report Date: June 5, 2018

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MEETING LOGISTICS

This report was prepared by the Born Qualified (BQ) Grand Challenge (GC) Laboratory Directed Research and Development (LDRD) External Advisory Board (EAB) for the following Sandia National Laboratories (SNL) personnel.

- Susan Seestrom, Advanced Science and Technology (AS&T) Associate Lab Director (ALD) and Chief Research Officer (CRO)
- Grant Heffelfinger, Deputy CRO Program Manager
- Greg Frye-Mason, LDRD and Academic Programs Manager
- Terry Aselage, BQGC Director Champion
- Shawn Dirk, BQGC Program Manager (PM)
- Allen Roach, BQGC Lead Principal Investigator (PI)
- GC Project Team members

The review meeting was held offsite on April 10 and 11, 2018, at SNL's Computer Science Research Institute (CSRI), conference room 90, Albuquerque, NM. A list of acronyms used in the report and a meeting agenda with briefing details are provided at the end of this report.

EXECUTIVE SUMMARY

The EAB concluded unanimously that Sandia should focus solely on two efforts in the remaining months of the Born Qualified Grand Challenge: Publish / communicate the results achieved to date (60% of remaining effort) and validate the models (40%). The results achieved to date are impressive, important, and need to be shared with the AM community. Publications are the first component of Sandia's outreach strategy; the second is a crisp articulation of how measurement, modeling and prediction come together to achieve qualification that can be adapted for multiple audiences.

The board strongly concurs that the project has produced clear benefit for Sandia. However, the benefit of this particular program to the Nation will be limited unless the findings can be broadly and effectively communicated. The timing of Sandia's BQ advances coincides ideally with a recent recognition at NNSA (NA-123) of the importance of innovation in non-nuclear materials and could do much to jump-start this program. The EAB would be pleased to share its assessment of these advances with NNSA if that would be appropriate and helpful.

The board commends Sandia for achieving a number of major accomplishments in this project:

- Establishing a strategy and roadmap that defined both the objectives of the Born Qualified project as well as the path beyond into aging and qualification.
- Focusing down on two exemplars (metal valve housing and ceramic ring), then bringing the LENS (Laser Engineered Net Shaping) process back in as an exemplar during the Demonstrator phase. The LENS process was a critical contributor to the project's modeling success, and, in our view, that process has been greatly revitalized as a result.
- Establishing a full suite of models across multiple-length scales, capable of passing data from one to another, along with an overarching methodology for associated uncertainty quantification (UQ) – this is a tremendous modeling achievement.
- Creating an Optimal Control strategy – a mathematically rigorous framework that incorporates the physics of the various phenomena being modeled.

Beyond the achievements in modeling and experiment, the EAB was impressed with Sandia's ability to "roll up the sleeves" and solve difficult practical problems such as focus and calibration issues. Perhaps Sandia should consider working with an agency like the National Institute of Standards and Technology (NIST) to establish Underwriter's Laboratory (UL)-like standards for machine performance. The EAB also recognizes Sandia's *al instante* high-throughput characterization and testing capability. The board is not aware of any other group having developed a comparable capability to generate significant quantities of high-quality data.

The most important capability generated by this project, however, is its development of future leaders in the field. The quality of their work has been outstanding. Our advice to these emerging leaders is that they should get out into the community, be recognized, and lead that community into the future.

The EAB sees great potential to further advance the Born Qualified work through the Digital Twin concept presented to us during lunch on the first day of the meeting. The approach is

unique to Sandia and its mission to understand the aging characteristics of components in the stockpile and begins to address the most difficult issue in qualification, which is how to predict and certify future performance.

EXTERNAL ADVISORY BOARD (EAB) MEMBERS

Members Present

- **Slade Gardner,** Acting EAB Chair, President, SG Advanced Manufacturing and Materials LLC
- **David L. McDowell**, Regents' Professor and Carter N. Paden Distinguished Chair in Metals Processing, Georgia Institute of Technology
- **David McMindes**, Chief Technology Officer, National Securities Campus (NSC), Honeywell Federal Manufacturing & Technologies, LLC. (Attended on Day 1)
- **William Tredway**, Associate Director for Advanced Manufacturing Technology, United Technologies Research Center

Members Absent

- **Craig Blue**, Director, Energy Efficiency and Renewable Energy Programs, Oak Ridge National Laboratory
- **Elizabeth Holm**, Professor of Materials Science and Engineering, Carnegie Mellon University

CHIEF RESEARCH OFFICER'S (CRO) CHARGE TO THE EAB

Thinking back to the beginning of the Born Qualified Grand Challenge and the accomplishments attained over the project's three-year duration, please help us assess overall performance and what has been achieved.

Born Qualified EAB – Meeting #4 Focus Questions	
Strategy	Has the GC team achieved measurable progress against its stated goals? What have been the most important accomplishments and shortcomings?
Relevance	Has the work provided clear benefit to Sandia and the Nation? How?
Quality	Has the team consistently demonstrated high-quality work throughout the project, and has that work been performed with high scientific integrity and fidelity? What advice for further improvement would you offer to future GCs at Sandia?
Capabilities	Has the project strengthened Sandia's technical base and produced clearly differentiated capabilities for the Lab? How?
Impact	Do you expect this project will have meaningful, long-term technical impact on component qualification (a) within Sandia and (b) upon the broader advanced manufacturing community? Why or why not?
In the remaining five months, what are the most important things the BQ team should focus on to maximize technical achievement and overall future impact?	

Five Elements of Research Assessment	
Strategy	Execute a research strategy that is clear, aligns discretionary investments (e.g., LDRD) with the research strategy, and supports DOE / NNSA priorities.
Mission and Impact Relevance	Ensure that research is relevant, enables the national security missions, and benefits DOE / NNSA and the nation.
Quality	Ensure that research is transformative, innovative, leading edge, high quality, and advances the frontiers of science and engineering.
Capabilities	Maintain a healthy and vibrant research environment that enhances technical workforce competencies and research capabilities.
Partnership & Technology Transitions	Research and develop high-impact technologies through effective partnerships and technology transfer mechanisms that support the laboratories' strategy and DOE / NNSA priorities and impact the public good.

EAB'S RESPONSE TO THE FIVE FOCUS AREAS

The EAB thanks Sandia for the opportunity to provide guidance to the Born Qualified Grand Challenge throughout the duration of the project. Our comments in response to the focus questions presented in the Charge are provided below.

Strategy	Has the GC team achieved measurable progress against its stated goals? What have been the most important accomplishments and shortcomings?
In the remaining five months, what are the most important things the BQ team should focus on to maximize technical achievement and overall future impact?	

The board begins its feedback with the final question posed in the Charge to the EAB regarding focus in the concluding months of the project.

The EAB concluded unanimously that Sandia should focus solely on two efforts in the remaining few months: Publish / communicate the results achieved to date (60%) and validate the models (40%). In making this recommendation, the board realizes how tempting it is to keep working to show "even better" results on the valve housing and ceramic ring exemplars – but also understands that doing so means that writing gets relegated to nights, weekends, or (in the worst case) after the project concludes when both time and money have vanished. The results achieved to date are impressive, important, and need to be shared with the AM community. SNL also risks missing out on critical recognition if publications are delayed and other groups report "piecemeal" individual findings similar to what Sandia has accomplished through this dedicated group effort. These publications form the first component of Sandia's outreach strategy.

The second component to outreach is the formulation of an "elevator speech" (which should include both three-minute and 30-second versions) that (a) succinctly summarizes how measurement, modeling, and prediction come together to achieve qualification, and (b) can be adapted for multiple audiences (OEMs, academic partners, program managers, etc.). While Sandia has assembled a vision that has worked admirably to manage this project and outline the Lab's future steps to the ultimate goal, an external listener needs to be a technical expert in many areas in order to comprehend it. Simplicity and clarity are paramount as Sandia carries its vision forward.

In addition to publishing / communicating results, the board likewise emphasizes validation of Sandia's various models as critical to continued funding, both internally from Sandia's weapons program and from external sources. We understand that DOE's Advanced Manufacturing Office (AMO) recently announced the availability of additional funds, which could be well suited to continuing Sandia's BQ efforts and for which Sandia, as a DOE entity, could be an attractive recipient.

Accomplishments:

The strategy and roadmap that defined both the objectives of the three-year Born Qualified GC project as well as the path beyond into aging and qualification is a major accomplishment. Although the project clearly outlined many ambitious goals at the beginning, the overall strategic element was missing and the team responded well when the EAB asked them to clearly define it. It is now apparent that this strategy served not only to organize the project, but also to drive Sandia's larger Additive Manufactuirng (AM) strategic plan.

The second major accomplishment was the team's decision to focus down from three exemplars to two (valve housing and ceramic ring) and then the decision to bring the LENS process back in as a third exemplar during the Demonstrator phase. The valve housing exemplar is an unqualified success, and the EAB was impressed with the creative thinking to determine how to build a better part with AM rather than simply attempting to duplicate the legacy part. The LENS process was a critical contributor to the project's modeling success, especially through its ability to monitor the melt pool *in situ* through the optical system. The Direct Write ceramic ring examplar, while less mature than the valve housing, also contributed significantly to the success of the project's modeling efforts.

The third major accomplishment is the actual suite of models across multiple length scales, capable of passing data from one to another, along with concepts and overarching methodology for associated uncertainty quantification. This is a tremendous modeling achievement. Lawrence Livermore National Lab (LLNL), for example, has a world-class model that exquisitely replicates physics at the molecular level, but it is not possible to translate results from this model up to the component level, which is what is ultimately required for qualification. Sandia adds uncertainty and performance margins to the multiscale model and experiment chain, which is a sigificant added value contribution (However, LLNL is very well known for this achievement and recognized as a leader, while Sandia labors in obscurity – a point that will be addressed again later in this report.)

The actual amount of data communicated across the models is not yet as significant as it will be downstream and will grow as models are exercised. As noted earlier, validation of the models is actually more critical to future success than immediately producing volumes of data.

At this meeting, the EAB saw the fourth major accomplishment – the Optimal Control strategy. We congratulate Sandia on creating a mathematically rigorous framework that incorporates the physics of the various phenomena being modeled. The approach is based on a governing set of differential field and constitutive equations; it would be useful to further incorporate the meta-models or surrogate models into that framework. In particular, phenomena and regimes of behavior for which the physical and chemical processes are less accurately addressed by present models can be addressed by approximate surrogate models within an Uncertainty Quantification (UQ) framework.

Beyond the achievements in modeling and experiment, the EAB was impressed with Sandia's ability to "roll up the sleeves" and solve difficult practical problems – for example, resolving the focus and calibration issues on the 3D Systems ProX 200 machine. Step-by-step instructions would benefit AM machine operators everywhere, and the availability of standardized machines, operated and maintained according to rigorous procedures, is key to the growth of AM – in

particular, DoD's future logistics vision. Perhaps Sandia could work with an agency like NIST to establish UL-like standards for machine performance and calibration ("Sandia Certified").

Shortcomings:

Given this list of accomplishments, the board felt that the project's shortcomings were relatively few. The EAB agrees with the team's realistic assessment provided in PI Allen Roach's concluding presentation. In the case of Optimization and Uncertainty Models, the most useful data sets came relatively late in the project, and less progress was made than initially hoped, but solid steps have been taken and the path forward is clear. In assessing the Multi-Scale, Multi-Physics Models, the EAB noted that passing data had been demonstrated, but actual quantiites have been limited; more effort is required here to demonstrate robustness.

The EAB expressed some disappointment that the Renishaw machines could not be brought online in time to produce data, both in quantity and in a form that would allow comparison to data produced on the same machines elsewhere in the NNSA complex. However, each of us also knows from personal experience that it often takes longer than planned to get machines installed and ready for reliable operation.

Relevance	Has the work provided clear benefit to Sandia and the Nation? How?

At this point, the EAB strongly concurs that the project has produced clear benefit for Sandia. An important accomplishment of this program is establishing the linkage between qualification based on performance margins, physically based multiscale modeling, and uncertainty quantification. This adds significant value which will benefit cross-cutting collaborations in future programs involving computational modeling, materials science, experimental methods, and UQ within Sandia. However, the benefit of this particular program to the Nation will be limited unless the findings can be broadly and effectively communicated. That is the basis for our recommendation that publications and outreach must be the #1 priority for the remainder of the project.

Rapid qualification is currently the hottest topic throughout the AM community, and there is general recognition that this issue must be solved for the technology to reach its full potential. The timing of Sandia's Born Qualified advances coincides ideally with a recent recognition at NNSA (NA-123) of the importance of innovation in non-nuclear materials and could do much to jump-start this program. As stated at the concluding Outbrief, one or more EAB members would be pleased to discuss the board's assessment of these advances with NNSA if that would be appropriate and helpful to both NNSA and Sandia.

Quality	Has the team consistently demonstrated high-quality work throughout the project, and has that work been performed with high scientific integrity and fidelity? What advice for further improvement would you offer to future GCs at Sandia?

The quality of the work has been outstanding – "top shelf, as we would have expected and demanded," in the words of one EAB member. Sandia is one of the few institutions in the world where the modeling work, in particular, could have been carried out at this scope and degree of integration. The inclusion of UQ across the entire effort is both a technical achievement and a cultural sign of the importance Sandia assigns to UQ. The EAB saw how this project made the modelers incorporate the physics of materials science, and in turn made experimentalists incorporate the tenets of UQ into their work. Future GC efforts at Sandia that include modeling and simulation should strive to integrate UQ at such a broad level.

Capabilities	Has the project strengthened Sandia's technical base and produced clearly differentiated capabilities for the Lab? How?

In addition to the list of differentiating capabilities already called out – the suite of models, the Optimal Control strategy, the deep understanding of processes and equipment, and UQ integration – the board adds the *Al Instante* high-throughput characterization and testing capability. The board is not aware of any other group having developed a comparable capability to generate significant quantities of high-quality data. This is especially important to the academic community, and we encourage Sandia to continue efforts to transfer these techniques to and to collaborate with appropriate partners.

Probably the most important capability generated by this project, however, is its growth of future leaders in the field. The EAB has been impressed by Sandia's staff across the board, from students to early career researchers to the senior members who have been mentoring them. We also commend the GC team management for the manner in which the work of so many talented people has been coordinated and kept on task.

Impact	Do you expect this project will have meaningful, long-term technical impact on component qualification (a) within Sandia and (b) upon the broader advanced manufacturing community? Why or why not?

The impact that this project will have is entirely in the hands of the team. The work has been done, the results have been outstanding, and all the pieces are in place waiting to be integrated

under the simplified statement of Sandia's strategy. As noted earlier, that strategy is sufficient for the continued advancement of Born Qualified within Sandia, but must be simplifed and communicated better in order to have external impact.

Our advice to the emerging leaders acknowledged above is that they should get out into the community, be recognized, and lead that community into the future. Take the opportunity to learn from the LLNL example and step into a highly recognizable role as Wayne King and his other colleagues have done. As this project has demonstrated, Sandia has performed leading-edge work on many fronts, and the institution will only be credited to the degree that each of its leaders is willing to step up. It is the right thing for Sandia and for the scientific community.

Although still in its early stages, the Optimal Control strategy has tremendous potential once Sandia starts applying it to practical problems. This project culminated in a sophisticated machine / process control strategy for AM that has significant potential to wrap in both physics-based models and surrogate-reduced-order models to describe various processes and process-structure-property mappings. The rigorous applied mathematics approach to UQ in this program is appreciated as a foundational starting point and can be evolved to accept meta-models based on experimental information, for example, as necessary to pursue overall systems qualification objectives. This will provide significant differentiation for this Sandia effort relative to current state of the art.

The EAB also sees great potential to further advance the Born Qualified work through the Digital Twin proposal described to us during lunch on the first day of the meeting. The approach is unique to Sandia and its mission to understand the aging characteristics of components in the stockpile. It also provides a means to inject new understanding of materials as it becomes available and begins to address the most difficult issue in qualification, which is how to predict and certify future performance. (What assurance do I have that this part will perform its intended function in 30 years?)

ADDITIONAL COMMENTS

Metals AM is among the most challenging problems with high potential payoff. The EAB congratulates the Sandia BQ team for keeping their eye on the "North Star" long-term objectives, moving all essential elements (modeling, experiment, UQ) together in unison toward that goal. In the spirit of a Grand Challenge LDRD, this is commendable and meets expectations of advancing the science and technology toward downstream applications.

At one point in the meeting, reference was made to a joint UTRC – GE – Honeywell project on distortion modeling under America Makes, and the question was raised how Sandia could access the relevant information. Presentations and reports produced during the project can be accessed by America Makes members via the organization's "Digital Storefront." Specific technical questions can be directed to Vijay Jagdale at UTRC (email: Vijay.Jagdale@utrc.utc.com; phone: 860-610-7186).

Acknowledgements

The EAB thanks Sandia's CRO, LDRD and GC leadership and team members for their advance preparations and briefings during the review. We also thank all who helped "behind the scenes" to organize this meeting and acknowledge Richard Macklin and Perspectives for its support to the EAB, especially in the preparation of this report.

Report date: June 5, 2018

APPENDIX A: NOMENCLATURE

Acronym	Definition
ALD	Associate Lab Director
AM	Additive Manufacturing
AMO	Advanced Manufacturing Office
AS&T	Advanced Science and Technology
BQ	Born Qualified
CRO	Chief Research Officer
CSRI	Computer Science Research Institute
DoD	Department of Defense
DOE	Department of Energy
EAB	External Advisory Board
GC	Grand Challenge
GE	General Electric
LDRD	Laboratory Directed Research and Development
LENS	Laser Engineered Net Shaping
LLNL	Lawrence Livermore National Laboratory
M&S	Modeling and Simulation
NIST	National Institute of Standards and Technology
NNSA	National Nuclear Security Administration
OEM	Original Equipment Manager
OUO	Official Use Only
PI	Principal Investigator
PM	Program Manager
S&T	Science and Technology
SNL	Sandia National Laboratories
UL	Underwriter's Laboratory
UQ	Uncertainty Quantification
UTRC	United Technologies Research Center

APPENDIX B: MEETING AGENDA

EAB Agenda – April 10
CSRI 90

Time	Topic	Speaker
8:00 – 8:15	Welcome & Charge for the Day	Terry Aselage
8:15 – 9:00	Opening Remarks & Sandia AM Overview	Shawn Dirk
9:00 – 9:30	Overview of Valve Housing Exemplar + Results	Kyle Allen
9:30 – 9:45	Break	
9:45 – 10:00	Valve Exemplar Plans to end of FY, Demonstrator 1A Results	Bradley Jared
10:00 – 10:30	Model Results - Part-scale Modeling of the Laser Powder Bed Fusion Process	Kyle Johnson
10:30 – 11:00	Overview of LENS Progress	Dave Keicher
11:00 – 11:30	LENS Modeling update	Mike Stender
11:30 – 12:30	Lunch	
12:30 – 12:45	Overview of Insulator Ring Exemplar	Dan Kammler
12:45 – 1:15	Insulator Ring Exemplar Plans to end of FY, Demonstrator 1A Results	Adam Cook
1:15 – 2:00	Insulator Ring Models	Brian Lester & Fadi Abdeljawad
2:00 – 3:30	Poster Session	
3:30 – 5:00	EAB Caucus/Questions/Discussion	

EAB Agenda – April 11
CSRI 90

Time	Topic	Speaker
8:00 – 8:15	Welcome, Review of Day 1	Allen Roach/Shawn Dirk
8:15 – 8:50	Integration, Optimal Control	Bart van Bloemen Waanders
8:50 – 9:10	Review of Data Progress and Challenges	Laura Swiler
9:10 – 9:50	Born Qualified Review	Allen Roach
9:50 – 11:00	EAB Caucus	
11:00 – Noon	Lunch, EAB Outbrief	Slade Gardner, EAB
Noon – 12:45	Lunch, Open Discussion	
12:45 – 1:00	Travel to AML	
1:00 – 2:30	AML Tour	Randy Schunk
2:30	Travel to Airport, Hotel	

Poster Session

1. Josh Stanford - Uncertainty Effects on mm-Wave and Infrared Temperature Measurement in Additive Manufacturing Applications
2. Amber Dressler - Mechanical Property Variation in Metal Lattice Struts
3. Andrew Kustas – High Entropy Alloys
4. Mark Wilson - Effects of elemental segregation during selective laser melting from atomistic simulations
5. Theron Rodgers – Microstructure Modeling for LENS and Powder Bed
6. Judy Brown - Challenges of Modelling Mechanical Behavior of Additively Manufactured Metals and Structures with Local Texture Variations
7. Samantha Taylor - Investigating Emissivity Dependence on Surface Roughness in Metal Additive Manufacturing
8. Erin Maines - Rheology of ceramic slurries for 3D printing using stereolithography
9. Matthew Roach – Challenges in SLA Printing of Ceramics
10. Dan Moser – Particle Scale Melt Modeling of Selective Laser Melting with Uncertainty Quantification

Note: The Alinstante video will be setup on the main screen and playing during the poster session

APPENDIX E: LISTING OF TOP PAPERS/PRESENTATIONS/INTELLECTUAL PROPERTY

1. R. Murphy, E. Forrest, J. Stanford, P. Woskov. "Calibration and Characterization of a Dual Millimeter-Wave Receiver High Temperature Measurement System." Review of Scientific Instruments. (In preparation)
2. S. Taylor, E. Forrest, J. Stanford. "Investigating Surface Roughness Effects on Emissivity for Metal Additive Parts." Annual International Solid Freeform Fabrication Symposium. Austin, TX. August 13-15, 2018.
3. J. Stanford, R. Murphy, and E. Forrest. "Microwave Thermal Analysis and Calibration for Additive Manufacturing." NCSLI 2017 Workshop & Symposium Exhibition. National Harbor, MD. August 14-17, 2017.
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