

*The National Academies of*  
SCIENCES • ENGINEERING • MEDICINE

**POLICY AND GLOBAL AFFAIRS**  
Board on International Scientific Organizations

**A Workshop on Predictive Theoretical and Computational Approaches for  
Additive Manufacturing**

Keck Center, Room K-100  
500 Fifth St. NW Washington, DC

**OCTOBER 7-9, 2015**

PROGRAM

This workshop will address challenges and opportunities in theoretical and computational methods to advance additive manufacturing (AM) in a holistic, multifaceted, and interdisciplinary way where experts from academia, national laboratories, and the private sector share their best practices and ideas to move forward. This workshop will focus in the following four areas: 1. Theoretical understanding of materials science and mechanics; 2. Computational and analytical methods in AM; 3. Monitoring and advanced diagnostics to enable AM fundamental understanding; 4. AM scalability, implementation, readiness, and transition. Over two days, experts will address a series of questions identified in the aforementioned four areas and also identify the necessary short-, intermediate-, and long-term goals to advance predictive methods in AM. Attendance is by invitation only, but remote viewers may watch the live webinar: <http://livestream.com/accounts/7036396/events/4350933>. A report will be produced afterwards summarizing the presentations and discussions of the workshop.

**Wednesday, October 7**

**Welcome – 8:00 a.m. (breakfast starting at 7:30 a.m.)**

**Wing Liu**, Chair of the U.S. National Committee on Theoretical and Applied Mechanics and Professor of Mechanical Engineering, Northwestern University (w-liu@northwestern.edu)

**Session 1: Theoretical understanding of materials science and mechanics – 8:15 a.m.**

Each expert will give a 25-minute presentation followed by a 30-minute discussion.

Theoretical understanding of materials science and mechanics, including related physical sciences, engineering, and mathematics, for additive manufacturing at all levels/stages. This includes but is not limited to design of metallic alloys or polymer blends, mixing and compatibilities of fundamental materials, heat (light) source interaction with feedstock, heat (light) source modeling, and incorporation of thermodynamic modeling into micro and macro heat transfer for the prediction of microstructures and metrology. Emphasis will be placed on polymers, alloys, and alloy-polymer interfaces.

## *Facilitator*

**Wing Liu**

## *Speakers*

**Marianne Francois**, Group Leader, XCP-4, Los Alamos National Laboratory ([mmfran@lanl.gov](mailto:mmfran@lanl.gov))

**Peter Olmsted**, Director of the Institute for Soft Matter Synthesis and Metrology, Georgetown University ([pdo7@georgetown.edu](mailto:pdo7@georgetown.edu))

**John Turner**, Group Leader, Computer Science and Mathematics, Oak Ridge National Laboratory, ([turnerja@ornl.gov](mailto:turnerja@ornl.gov))

### Questions to be addressed:

- (1) What are the fundamental scientific (AM) issues that should be addressed in this workshop?
- (2) What are the unique fundamental theoretical and computational approaches that need to be proposed and developed to fully understand AM?
- (3) What are the mathematical models and state-of-the-art theoretical, computational simulation models that describe the different aspects of AM, and what new methods (computational, statistical, experimental consistent) are needed to simulate the various stages of AM?
- (4) What integration frameworks currently exist for coupling these modeling techniques together to advance AM to the next stage of maturity?
- (5) What are the most important open questions in materials and mechanics, including related scientific disciplines, engineering and mathematics, as well as the technical challenges to be addressed for predictive theoretical and computational approaches in order to enable widespread adoption of additive manufacturing?
- (6) Does AM require unique fundamental research in theoretical and computational materials science, mechanics and multi-scale computation? What are the opportunities?
- (7) What multidisciplinary and related materials and mechanical sciences are needed for AM?
- (8) How will theoretical and computational models be validated/verified for a particular or a generic AM process (intermediate steps or complete AM result)?
- (9) What opportunities exist for public-private partnerships to advance theoretical and computational mechanics capabilities for AM?
- (10) How will those partnerships benefit from advancements?
- (11) Do materials standards change with a Theoretical and Computations approach to materials development and implementation?

*10:00 a.m. – BREAK (15 minutes)*

## **Session 2: Computational and analytical methods in AM – 10:15 a.m.**

Each expert will give a 25-minute presentation followed by a 30-minute discussion.

Novel computational and analytical methods for fully characterizing process-structure-property relations in additive manufacturing (AM) processes for materials design, product design, part qualification, and discovery/innovation such as multi-scale modeling, computational materials, topology optimization, verification and validation methods, and uncertainty quantification for AM processes and AM resulting materials, etc.

## *Facilitator*

**Steve Daniewicz**

## *Speakers*

**Corbett Battaile**, Materials and Process Modeling Department, Sandia National Laboratories  
([ccbatta@sandia.gov](mailto:ccbatta@sandia.gov))

**Wayne King**, Director, Accelerated Certification of Additively Manufactured Metals Initiative, Lawrence Livermore National Laboratory ([weking@llnl.gov](mailto:weking@llnl.gov))

**Anthony Rollet**, Professor, Materials Science and Engineering Department, Carnegie Mellon University  
([rollett@cmu.edu](mailto:rollett@cmu.edu))

### Questions to be addressed:

- (1) Computational methods and approaches for simulating materials processing, properties and performance relationships for materials design using additive manufacturing as well as key process parameter identification and process mechanics.
- (2) How to leverage high performance computing spanning scientific discovery to ensembles of engineering solutions?
- (3) How to integrate topological design loops with additive manufacturing processes and mechanics within a computational framework?
- (4) How can AM benefit from fundamental advances in verification, validation and uncertainty quantification methodologies? (Prelude to In-Situ Monitoring & Diagnostics theme)
- (5) What analytical, experimental, and software tools are needed?
- (6) How can these be integrated to impact adoption of AM? (Transition to scalability theme)
- (7) What opportunities exist for high performance computing, in order to provide fundamental scientific discovery of the process-properties-performance relationship relevant to AM?
- (8) What are those drivers and what fundamental advancements are needed for computational methods and optimization techniques?

*12:00 p.m. – LUNCH provided*

## **Session 3: Monitoring and advanced diagnostics to enable AM fundamental understanding – 1:15 p.m.**

Each expert will give a 25-minute presentation followed by a 30-minute discussion.

In-situ monitoring and advanced diagnostics to enable AM fundamental understanding (for example metrology). Additive manufacturing provides a fundamentally different way to build components, as opposed to subtractive manufacturing. Typically, in subtractive manufacturing, metrology is executed after all material is removed, as this is when the part receives its final shape. With AM, metrology can occur during the process and corrective actions can be taken in-situ. It is expected that in-process metrology will not provide a binary (go/no-go) result, but a probabilistic result (quantifying quality/conformance uncertainty). Thus, the concept of metrology for AM will be interpreted and represented differently than classical metrology. Furthermore, AM processes offer the opportunity to quantify errors and correct them in-process by incorporating sensors other than dimensional, resulting in significantly different closed-loop process control systems. AM enables the manufacture of multi-material, and functionally graded material components. Such a capability will require a new set of in process sensor tools to validate material quality, composition and key performance parameters.

## *Facilitator*

**Tony Decarmine**

## *Speakers*

**Joseph Beaman**, Professor, Mechanical Engineering Department, University of Texas-Austin  
([jbeaman@mail.utexas.edu](mailto:jbeaman@mail.utexas.edu))

**Jian Cao**, Professor of Mechanical Engineering and Director of the Initiative for Manufacturing Science and Innovation, Northwestern University ([jcao@northwestern.edu](mailto:jcao@northwestern.edu))

**Ade Makinde**, Principal Engineer, GE Global Research Center ([makinde@ge.com](mailto:makinde@ge.com))

### Questions to be addressed:

- (1) What are the in-situ and/or diagnostics challenges specific to AM?
- (2) What new types of diagnostics/sensors are required to probe the AM fabricated materials?
- (3) What recent advances in experimental methods can be leveraged to achieve this?
- (4) What new in-situ and/or diagnostics methods need to be developed?
- (5) Where are we deficient now?
- (6) How do we integrate uncertainty analysis into the process monitoring and diagnostics capabilities?
- (7) Given that AM enables the realization of both design geometry and multi-material characteristics, how do we develop digitally compatible computational and design tools that address and integrate multi-material and geometric information into the functional design and manufacturing process?
- (8) How else can the overall data collected during the in-situ measurements be used for design iteration, analysis (re-analysis) inputs, optimization, quality assessments and post product delivery?

3:00 p.m. – BREAK (30 minutes)

## **Session 4: AM Scalability, Implementation, Readiness, and Transition – 3:30 p.m.**

Each expert will give a 25-minute presentation followed by a 30-minute discussion.

Additive Manufacturing Scalability/Implementation/Readiness/Transition including fundamental bridges that must be forged to take analytical, computational, and mechanistic models and initial laboratory experiments into pilot production lines, and subsequently into full scale production for rate, quantity and size considering mass customization theme.

## *Facilitator*

**Slade Gardner**

## *Speakers*

**Anthony (Tony) DeCarmine**, Chief Technology Officer, Oxford Performance Materials  
([tdecarmine@oxfordpm.com](mailto:tdecarmine@oxfordpm.com))

**Lyle E. Levine**, Staffer, Materials Science and Engineering Laboratory, National Institute of Standards and Technology ([lyle.levine@nist.gov](mailto:lyle.levine@nist.gov))

**Yung Shin**, Professor, Advanced Manufacturing, Purdue University ([shin@purdue.edu](mailto:shin@purdue.edu))

### Questions/Issues to be addressed:

- (1) What is the path for utilizing fundamental results for AM and scaling them for use in productions?
- (2) What are the roadblocks that hinder the scaling of AM technologies into production and use in systems?
- (3) Do any of these roadblocks represent problems/issues that can be best addressed through additional fundamental research?

- (4) What are future applications, markets and industry partners that may leverage the fundamental research and scale it into production?
- (5) What measurements of quality or systems are appropriate that correlate computational and analytical methods to practical implementation?
- (6) Software architecture and data-bases for AM model development
- (7) Careful design of validation experiments for model validation, uncertainty quantification, and in situ process monitoring
- (8) Software development, integration with precision engineering, and integration into engineering work flow
- (9) Are there drivers to integrate computational simulation and advanced optimization methodologies to enable unique AM design?
- (10) What opportunities exist for public-private-partnerships to advance HPC capabilities for AM?
- (11) How will those partnerships benefit from advancements?
- (12) Do processing standards change with an analytical and mechanistic model approach to implementation of full scale additive manufacturing?

5:15 p.m. – ADJOURN

**Thursday, October 8**  
**(breakfast starting at 7:30 a.m.)**

**Session 5: Theoretical understanding of materials science and mechanics – 8:00 a.m.**

Each expert will give a 25-minute presentation followed by a 30-minute discussion where they will continue addressing the questions from Session 1.

*Facilitator*

Wing Liu

*Speakers*

**Steve Daniewicz**, Professor, Mechanical Engineering Department, Mississippi State University  
([daniewicz@me.msstate.edu](mailto:daniewicz@me.msstate.edu))

**Neil Hodge**, Solid Mechanics and Code Developer, Methods Development Group, Lawrence Livermore National Laboratory ([hodge3@llnl.gov](mailto:hodge3@llnl.gov))

**Saad Khairallah**, Computational Engineer, Computational Engineering Division, Lawrence Livermore National Laboratory ([khairallah1@llnl.gov](mailto:khairallah1@llnl.gov))

9:45 a.m. – BREAK (30 minutes)

**Session 6: Computational and analytical methods in AM – 10:15 a.m.**

Each expert will give a 25-minute presentation followed by a 30-minute discussion where they will continue addressing the questions from Session 2.

*Facilitator*

Steve Daniewicz

### *Speakers*

**Joe Bishop**, Computational Structural Mechanics and Applications, Sandia National Laboratories  
([jebisho@sandia.gov](mailto:jebisho@sandia.gov))

**David Snyder**, Sr. Materials Development Engineer, QuesTek Innovations ([dsnyder@questek.com](mailto:dsnyder@questek.com))

**Gregory Wagner**, Associate Professor, Mechanical Engineering, Northwestern University  
([gregory.wagner@northwestern.edu](mailto:gregory.wagner@northwestern.edu))

*12:00 p.m. – LUNCH provided*

## **Session 7: Monitoring and advanced diagnostics to enable AM fundamental understanding – 1:15 p.m.**

Each expert will give a 25-minute presentation followed by a 30-minute discussion where they will continue addressing the questions from Session 3.

### *Facilitator*

**Slade Gardner**

### *Speakers*

**Dave Keicher**, Optomec Founder, Senior Member of Technical Staff – Sandia National Laboratories  
([dmkeich@sandia.gov](mailto:dmkeich@sandia.gov))

**Eddie Schwalbach**, Research Materials Engineer, Air Force Research Laboratory ([edwin.schwalbach@us.af.mil](mailto:edwin.schwalbach@us.af.mil))

**Yu-Ping Yang**, Modeling Engineer, EWI ([yyang@ewi.org](mailto:yyang@ewi.org))

*3:00 p.m. – BREAK (30 minutes)*

## **Session 8: AM Scalability, Implementation, Readiness, and Transition – 3:30 p.m.**

Each expert will give a 25-minute presentation followed by a 30-minute discussion where they will continue addressing the questions from Session 4.

### *Facilitator*

**Tony Decarmine**

### *Speakers*

**Tahany El-Wardany**, Fellow, Physical Science Department, United Technologies Research Center  
([ElWardTI@utrc.utc.com](mailto:ElWardTI@utrc.utc.com))

**Rainer Hebert**, Associate Professor at the Department of Materials Science & Engineering and Director of Additive Manufacturing Innovation Center, University of Connecticut ([rhebert@ims.uconn.edu](mailto:rhebert@ims.uconn.edu))

**Alonso Peralta-Duran**, Honeywell International Inc. ([alonso.peralta@honeywell.com](mailto:alonso.peralta@honeywell.com))

*5:15 p.m. – ADJOURN*

## **Friday, October 9**

### **Session 9: Reflections – 8:30 a.m. (breakfast starting at 8:00 a.m.)**

Speakers from each session and attendees will meet separately (in the atrium) to discuss whether their questions have been addressed and to formulate questions that are still unanswered. They will reflect upon the last couple of days. They will also discuss what they would like to see as follow-up to the workshop.

#### *Facilitators*

**Steve Daniewicz**

**Topic - Theoretical understanding of materials science and mechanics**

**Wing Liu**

**Topic - Computational and analytical methods in AM**

**Jian Cao**

**Topic - Monitoring and advanced diagnostics to enable AM fundamental understanding**

**Tony Decarmine**

**Topic - AM Scalability, Implementation, Readiness, and Transition**

### **Session 10: Closing session – 10 a.m.**

#### *Facilitators*

**Wing Liu and Tony Decarmine**

- (a) Reflections of each session (1 speaker/session)
- (b) Each group presents its ideas about follow-up
- (c) Closing discussion.

*Noon – ADJOURN*