The National Academies of
SCIENCES • ENGINEERING • MEDICINE

Defense Materials Manufacturing and its Infrastructure (DMMI)

Workshop on:

Data analytics and what it means to the Materials Community

National Academy of Sciences building, July 16 - 17th 2019,
Room NAS120 at 2101 Constitution Avenue, NW.

The Academies will convene a workshop to discuss issues in defense materials and manufacturing. The topics to be discussed is Data analytics and what it means to the Materials Community.

The following abstract will define the workshop:

The 2013 NRC report on "Frontiers in Massive Data Analysis" makes the following statements about big data: "Experiments, observations, and numerical simulations in many areas of science and business are currently generating terabytes of data, and in some cases are on the verge of generating petabytes and beyond. Analyses of the information contained in these data sets have already led to major breakthroughs in fields ranging from genomics to astronomy and high-energy physics and to the development of new information-based industries." Traditionally, in materials research a deterministic approach have been used to uncover mechanisms of observed behavior and to make predictions. A question that becomes obvious is: To what extent today, can one use informatics for materials research challenges and discover unexpected correlations by analyzing huge data sets to find relationships that were not anticipated? Another question is how could these insights help to guide experimentation in future materials research efforts? These, and related questions will be discussed in this workshop.

July 16, 2019

OPEN SESSION

8:00 Working Breakfast

8:30 Welcome, Meeting Objective, Introductions – CHAIR **Haydn Wadley**

8:45 **Keynote Speaker Gareth Conduit,** Intellegens
Presentation title: *Data analytics and what it means to the Materials Community*

Topic 1: Materials Design

Introductions by: Lourdes Salamanca-Riba Q&A conducted by: Tresa Pollock

9:35 **Speaker Bill Mahoney**, ASM International
Presentation title: *Data Analytics in the ASM community*

10:05 Break

10:25 **Speaker Chris Wolverton,** Northwestern
Presentation title: *Materials Design today*

10:55 **Speaker Steven Arnold**, NASA
Presentation title: *NASA and current materials development*

11:25 Lunch

12:25 **Panel Discussion on *Materials Design***

Introductions by: Tresa Pollock Q&A conducted by: Lourdes Salamanca-Riba

Panelists: John Mauro, Penn State
Panelists: Brian Storey, Olin College & Toyota Res. Inst.
Panelists: Dane Morgan, U. of Wisconsin-Madison

Topic 2: Data Curation

Introductions by: Robert Hull Q&A conducted by: Susan Sinnott

01:45 **Speaker James Goddin,** ANSYS Granta (Zoom)
Presentation title: *Data Management and Machine Learning aspects of the Accelerated Metallurgy project.*

2:15 **Speaker Josh Peek**, Space Telescope Science Institute
Presentation title: *Toward a Grand Unified Practice of Astronomical Metadata*

2:45 Break

3:00 **Speaker Marty Green**, NIST
Presentation title: *Next Generation Materials Genome Initiative (MGI), Driven by Data and Artificial Intelligence*

3:30 **Panel Discussion on Data Curation**

Introductions by: Susan Sinnott Q&A conducted by: Robert Hull

Panelists: B.S. Manjunath, UC Santa Barbara
Panelists: Ichiro Takeuchi, U. of Maryland
Panelists: Cormac Toher, Duke

4:50 Wrap up and final comments

5:00 Adjourn meeting day 1

July 17, 2019

OPEN SESSION

8:00 Working Breakfast

8:30 Welcome, plans for today – **CHAIR Haydn Wadley**

8:45 **Keynote Speaker Surya Kalidindi**, Georgia Tech
Presentation title: *AI-Based Knowledge Systems for Supporting Materials-Manufacturing Innovations*

Topic 3: Emerging Applications

Introductions by: Haydn Wadley Q&A conducted by: Ward Plummer

9:35 **Speaker Apurva Mehta,** Stanford
Presentation title: *Accelerating discoveries of compositionally complex alloys by iterating machine-learning with high throughput experimentation*

10:05 Break

10:25 **Speaker Florencia Paredes**, Citrine.io
Presentation title: *Challenges and Opportunities of Applying AI to Materials Data*

10:55 **Speaker Carla P. Gomes**, Cornell
Presentation title: *What the future holds*

11:25 Lunch

12:25 **Panel Discussion on *Grand Challenges for the Future***

Introductions by: Ward Plummer Q&A conducted by: Haydn Wadley

Panelists: Gareth Conduit, Intellegens
Panelists: John Gardner, NASA
Panelists: Jim Warren, NIST

1:45 **Wrap up discussion for the full workshop**

2:30 **Adjourn meeting**

3:00 (planning committee and Reliance only) **Call regarding future topic order**

4:00 (planning committee and Reliance only) **Adjourn fully**

For more information contact:

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Future Schedule

The future DMMI workshop schedule is as follows (Save the dates):

2019 November	19-20	D.C., NAS building, room 120
2020 March	17-18	D.C., Keck Building, Room 208
2020 July	14-15	D.C., Keck Building, Room 208
2020 November	17-18	D.C., Keck Building, Room 208

Future Topics

The upcoming five topics are (not in order):

- Domestic manufacturing capabilities: Emerging Needs in Quantum-enabled systems (March 19-20)
- Data analytics and what it means to the Materials Community (July 16-17)
- **Topology Optimization in Design: Exploiting Advanced Manufacturing Capabilities (Nov. 19-20)**
- What's next after CMOS? (order not set)
- What does quantum computing bring to new materials design? (order not set)

Expanded Future Topics

Topology Optimization in Design: Exploiting Advanced Manufacturing Capabilities

Topological Optimization (TO), i.e. optimizing the layout of material in a design space, has become computationally practical, and offers new possibilities for integrating design of materials and design of products to take full advantage of advanced manufacturing (especially additive manufacturing). Success stories abound using TO to produce non-intuitive designs that minimize weight in structural components, and the technique has been used to optimize for unusual and often DoD specific needs and models, such as burn rate of propellants for rocket grain. Extending TO beyond shape optimization offers the possibility of designing and analyzing gradient material structures that can be built with additive manufacturing materials and methods. At the system level, TO offers a way to rapidly explore design trade spaces and generate designs that respond quickly to changes in needs. The combination of TO and additive manufacturing can bring production systems close to the vision of Agile Manufacturing, formulated in 1991 as “the ability to thrive on change”. This workshop will examine how TO can be effectively implemented and extended to meet next generation needs in defense manufacturing, and explore alternatives for unifying its use in materials and manufacturing communities..

What's next after CMOS?

Both classical and quantum computing face significant challenges. On the classical side, silicon field effect transistors are reaching the fundamental limits of scaling and there is no replacement technology which has yet demonstrated even comparable performance to the current generation of commercially available silicon CMOS. On the quantum side, scaling the number of entangled superconducting or trapped ion qubits to that required to solve useful problems is an enormous challenge with current device technology. Both fields stand to benefit from transformational devices based on new physical phenomena, new materials, and new fabrication and manufacturing processes. While much attention has been given to these issues separately, the research must be both significant and coordinated among those with expertise in theoretical solid-state physics, quantum transport measurements, ultrafast optical spectroscopy, novel device engineering, electronic device processing, computational materials science, materials growth, materials fabrication, and advanced packaging. In this workshop, the issues at the convergence of these disciplines will be explored with the stakeholder communities involved.

What does quantum computing bring to new materials design?

Fundamental transformations in the basic logic of computing are few and far between. However, today the materials research community is actively discussing the potential for quantum computing to apply such a transformation in materials and chemistry discovery. The ultimate goal in the materials research community is to synthesize new materials with desired properties in a controlled way via materials engineering modeling starting at the atomic scale, and extending to macro scales. These models are computationally limited even when implemented on the most capable supercomputers to date. It is believed that quantum computing can speed up the computation process, and, perhaps more importantly, support algorithmic approaches that uniquely fit the needs of multi-scale materials design. Quantum computers in the laboratory are built with an increasing number of qubits. At a few hundred qubits, materials research challenges will become possible to tackle. It is now time to better understand not only how algorithms are being developed for materials discovery, but also how materials science principles can be incorporated into the discovery and design tools that may emerge. This workshop will address the fundamental differences in quantum computing from today's algorithms, the principles that might be used to develop future algorithms suited to materials engineering, expected gains in computational speed and efficiency, and what topics might be attempted to be analyzed first.