Accelerating Translational Materials R&D for Global Challenges

NSF Convergence Accelerator Virtual Workshop

Final Report

May 17 - June 1 2021

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Executive Summary

Materials science holds great promise for addressing urgent global challenges in climate, energy, health, and sustainability. Advances in material science will be critical for problems such as designing effective carbon capture for emissions, achieving high energy density, safety, and sustainability of battery technologies, enabling rapid design of therapeutics, and creating new materials for purification of water. While fundamental advances in materials science are required through continued basic research, new focus is needed to shepherd innovations from the laboratory through development, qualification, scale-up, lifecycle analysis, deployment, use, and to provide continuous feedback to achieve real-world impact. Particularly, in an emerging era of accelerated scientific discovery where faster progress is being made in science, new focus is needed to remove bottlenecks for rapidly translating new scientific knowledge to impact. Such a translational effort is inherently convergent, requiring a diversity both of stakeholders and of technical expertise, and is consistent with the objectives of the NSF Convergence Accelerator program. This workshop brought together experts from the materials science community to identify barriers to translation and propose possible solutions. A key 3-year milestone was identified in each of five technical areas:

1. **Materials Research Data Sharing Principles & Infrastructure:** Establishment of a common US-wide data standard and data sharing infrastructure for academic, government, and industrial materials data, building on FAIR data principles[1] and providing needed metadata, annotations, and access controls.
2. **Incentives for Long-term Investment & Sustainability:** Creation of a multi-stakeholder effort that demonstrates the effective use of a convergence approach to de-risk solutions in an area of sustainable materials, such as polymers.
3. **Full-lifecycle and Sustainability "Systems Thinking" in Materials Design:** Demonstration of an open data platform and program for holistic materials research and development that incorporates interdisciplinary perspectives beyond materials science (lifecycle analysis, socio-economics, policy, environmental issues, &c.) in an area with large societal impact like materials for the built environment.
4. **Construction of Inclusive, Large-scale Partner Ecosystems:** Implementation and evaluation of multiple embedding mechanisms (collaboration, technology transfer, internships, sabbaticals, visiting scientists, &c.) to see which are most effective at building strong, inclusive communities of innovation that connect materials science and manufacturing.
5. **Making Materials Knowledge Consumable in Design and Manufacturing:** Demonstration of programs that drive enhanced data sharing between academic materials research and industry in the form of student projects, industrial internships, and joint training.

As noted above, the challenge of effectively connecting materials discovery and design to production manufacturing was highlighted in multiple threads of the workshop. Academic researchers do not feel they have the needed information or access to understand practical

materials problems in manufacturing, sustainability, or lifecycle analysis, and manufacturing experts do not feel they can engage effectively with materials researchers given short-term timescales and the need to keep data or methods proprietary. Both communities recognize the benefits of interacting, yet are constrained by their immediate incentives. This is intrinsically a multi-disciplinary, multi-party, complex problem that calls out for a convergent approach from NSF. Integrating the feedback from the workshop participants, NSF could take high-level actions such as:

- Creation of a new NSF Convergence Accelerator program focused on the multi-disciplinary, multi-stakeholder challenge of speeding up the translation of new sustainable materials concepts from basic research to manufacturing, while obtaining continuous feedback of needs to allow more agile approaches for fundamental science.
- Integration of a Convergence Accelerator program with existing cross-agency efforts like the Materials Genome Initiative and particularly the Manufacturing USA Institutes to inform and implement this accelerated translation.

Beyond the technical domain of materials science, broader high-level convergence recommendations from the workshop for NSF action include:

- Re-imagining the existing US intellectual property framework through a multi-stakeholder program that recommends a roadmap of changes.
- Development of a "materials data librarian" career path to support the general-purpose but specialized skills required to collect, organize, structure, share, and maintain scientific data relevant for chemical and materials R&D. The field of library science includes representative expertise, but it needs to be developed as a profession in the context of materials.
- Creation of simple, low-overhead mechanisms enabling easy sharing of industrial challenges with academic researchers, undergraduate/masters student project-based learning or capstone projects to address those challenges, and implementation of the results in industry without loss of competitive advantage.
- Implementation of use-focused convergence teams in specified application areas to develop 1-3 year shared efforts and associated milestones to impact global challenges.

Workshop Summary

The NSF Convergence Accelerator Workshop "Accelerating Translational Materials R&D for Global Challenges" was a fully virtual workshop with an introduction/tech support session on Friday May 17 followed by three three-hour interactive ideation sessions on May 20, 24, and June 1. The workshop brought together a diverse collection of 57 researchers across the materials community, spanning academia, startups, industry, and non-profits as well as technical areas including materials discovery, materials informatics, sustainability, scale-up, and manufacturing. A specific goal of the workshop was to ask the question "if we can speed materials discovery by 2-10x, thanks to the past decade of research investments such as the Materials Genome Initiative, what's the next bottleneck, and can it be addressed with a convergence approach?"

This workshop built on two prior Convergence Accelerator workshops: "Design for a Circular Economy from Molecules to the Built Environment"[2] and "Socioresilient Infrastructure: Precision Materials, Assemblages, and Systems"[3]. The connections and synergies between these three workshops are highlighted in the main report. In addition, the workshop was directly connected to the NSF "Industry-Academia Collaboration in Advanced Manufacturing"[4] workshop with a shared panel discussion at the end of the first full workshop day.

The participants identified ~175 different questions, challenges, and impediments to effective translation of materials R&D to impact. These were summarized and the 5 key themes generated, validated, and explored in depth by workshop participants were:

1. Materials Research Data Sharing Principles & Infrastructure
2. Incentives for Long-term Investment & Sustainability
3. Full-lifecycle and Sustainability "Systems Thinking" in Materials Design
4. Construction of Inclusive, Large-scale Partner Ecosystems
5. Making Materials Knowledge Consumable in Design and Manufacturing

For each topic, a team of 5-6 participants generated a problem description, value statement, and completed a visualization exercise to propose candidate formations of convergent teams that could advance the topic, identifying participant archetypes, structured milestones, and connections to other initiatives and funding agencies. Some of the materials areas identified by participants as ripe for innovation included sustainable/recyclable polymers, additive manufacturing, biopolymers, micro-structured materials, future energy solutions, and benign decomposition. It was broadly felt that investments in these areas could help address urgent challenges related to climate, energy, water, and health, advance skills of the workforce and create jobs, and drive the US economy.

However, key organizational challenges were identified for translation of materials innovation, which include: the gap between basic research (e.g., academic discovery focused on single properties vs. multi-property needs in manufacturing), disparate professional timescales across research, manufacturing and deployment, misalignment of incentives and differences in culture, costs of lifecycle analysis, feedstock availability, and the need for specific policy and program support for long-term translation efforts. Interesting workforce and training elements were identified — specifically, the need for trained "data managers/archivists" to facilitate data sharing, the need to enable small-scale and short-timescale industry-defined projects for undergraduate (particularly PUI) education, and the emergence of a small population of researchers with skills bridging multiple materials areas (simulation, fabrication, experiment, development) who might serve as archetypes for future education.

Participants generally agreed that addressing any of these areas will require a multi-stakeholder multi-disciplinary approach, with careful attention paid to the different decision timescales and incentives. There was also agreement that the global challenges addressed by materials are urgent and growing more so every day. The remarkable speed with which the biomedical community was able to respond to a pandemic, building on decades of sustained NIH and NSF investment, was highlighted as an inspiration and a motivation to build similar materials capabilities to address other pressing global challenges.

Practical aspects of the workshop:

The workshop was carried out with the help of KnowInnovation, a conference facilitator that has successfully worked on prior NSF workshops. The KnowInnovation team helped with agenda planning, the conference website, registration, attendee reminders, workshop facilitation, and operations during the workshop sessions.

Demographic details of workshop participants were collected by KnowInnovation and shared directly with NSF. A detailed list of workshop attendees is included below in Appendix 1.

The workshop included a formal code of conduct, which each participant had to acknowledge as part of the registration process. The specific language of the code of conduct, adapted for a virtual workshop, was:

> Our workshop is dedicated to providing a harassment-free workshop experience for everyone, regardless of gender, gender identity and expression, age, sexual orientation, disability, physical appearance, body size, race, ethnicity, religion (or lack thereof), genetics, or technology choices. We do not tolerate harassment of workshop participants in any form.
>
> Harassing language or content is not appropriate for any workshop venue, including but not limited to virtual sessions, talks, preparation sessions, breakout sessions, working groups outside the main workshop, or social media. Workshop participants violating these rules may be sanctioned or expelled from the workshop without appeal *and their behavior reported to their home institution and the National Science Foundation.*

Given the necessarily virtual nature of the workshop, the organizing team decided to explore a "flipped workshop" approach inspired by the "flipped classroom" model in general education. The "flipped classroom" model moves explanatory lectures from in-person to recorded pre-work for each classroom session and reserves the actual classroom time for in-person interaction. In a traditional scientific workshop or conference, most of the workshop time is spent in formal presentations, limiting the time for interactive discussion.

For this workshop, the organizing team recorded multiple presentations from invited speakers that were assigned as the pre-work for each workshop session (see Appendix 2). Participants were asked to watch these recordings independently, and bring any insights or ideas sparked by the speakers to the session. This allowed us to preserve the workshop session time for ideation (see Appendix 3) and small group interaction.

In retrospect, one recommendation for future workshops using this model would be to start each session with an interactive Q&A panel discussion with the recorded speakers. We did this in the first session of the workshop and it increased engagement with the participants, but did not have time to include such a Q&A in subsequent sessions.

Pre-interviews with workshop participants:

Prior to the workshop convening we conducted interviews with nine registered workshop members. Our interview participants came from three distinct sectors of the translational materials ecosystem: three from the industry, four from academia, two from regulatory agencies. All interviews were conducted in a one-on-one setting with Dr. Gemma Jiang, the social scientist on the workshop organizing committee.

We had two clear intentions for the interviews:

The first was to get to know our participants in depth and personally. In this vein, we asked questions about the workshop specifically, such as: What attracted you to the workshop? What are your expectations? What are you looking to take away from the workshop? We also included questions about their own general experiences with the translational materials ecosystem like: What are the fragmentations and silos can you personally identify? What are your own stories of success and what challenges you face working across silos?

The second was to communicate workshop expectations from the organizing committee. We shared expected mindsets, such as openness to the unknown, ecosystem awareness, and recommended behaviors, such as using plain language, being present and engaged, suspending judgement, and reframing problems as questions.

Below is a summary of the themes that emerged from the interviews with supporting quotes.

Theme 1. We will reap concrete benefits by engaging in cross-sector collaboration.

It is a long journey from research labs to real world impact, and many sectors are involved in the process. To define challenges worthy of funding, we need a microcosm of the ecosystem. Interviewees also identified concrete benefits, such as sharing facilities and talents.

Below are some relevant quotes.

- “Work together to identify appropriately scaled and technically feasible challenges. I do not think one person can be sufficiently expert in all these things.”
- “Academics have not had to think about material design in a global complex way.”

- "Remote control experiments, a series of academic experiments can be conducted at other facilities. Just the beginning of these unlimited possibilities for academic-industry partnership."
- "Academic benefit from partnership with industry: Access to real world challenges, insights beyond textbook knowledge. If you do not have the insight, you may not even know what problems to solve. Scale of the problem, potential promising field, and some of the big technical challenges."
- "Industry benefits from partnership with academics: Creativity, and openness in the solution space, unrestricted view, search for novelty. Industry is much more confined and more streamlined, less crazy ideas, and the "crazy ideas" might open up new fields. Also, diversity, depends on how you set up the collaboration, partners more complementary to each other, access to domain knowledge you may not have. How impact papers come to be, bring together different fields and you have a new way of making (e.g. 3D printing human organs)."

Theme 2. We need to pay special attention to key connection points in the ecosystem.

Interviewees called attention to the following key connection points in the ecosystem: research and development, production, scale up, market response, public perception, regulatory framework, and energy landscape.

Below are some relevant quotes.

- "We have a strong need to strengthen the connection between material/data scientists, economists and decision makers."
- "I represent the scientists 'worst nightmare'. I can be the "reality checker". I bridge the divide between upstream (people who develop technology) and downstream (people who assess and regulate technology). Get early signals from downstream people to reduce risk and build trust. Bad news is good as long as it is early."
- "What is the right handover point between R&D and production? How far do you have to go in a research project to hand over to industry? There are a lot of difficulties in the transition to production. Somebody who developed the materials shows it is possible, but other people have never worked on the process. The next challenge is if you want to scale up a material, you have to make sure it is something customers want to buy. I also see the impact of the regulatory framework, such as carbon pricing. Why would you want to invest in this kind of uncertainty when nobody knows the future of the energy landscape?"

Theme 3. There is demonstrated enthusiasm as well as identified challenges for data scientists and computer scientists to work together.

Interviewees acknowledged the success over the past decades to break down silos in the materials innovation ecosystem. Specific challenges the community face right now include quantity of data in empirical vs computational methods, difference in culture (e.g. hypothesis driven vs empirical driven); unifying principles vs domain specific expertise.

Below are some relevant quotes.

- "We need very fast changes in materials innovation, but we are suffering from the long time it takes to get to market. We see emerging tools like data science, but not enough of a unified vision."
- "There is a lot of hype when AI is involved. Some people manipulate a problem in materials science to fit AI. I am interested in using these methods to deliver real world impact."
- "Material science domains themselves are siloed. We have genetic techniques in machine learning, the math and algorithms are the same (unifying principles), but different domains of material science may have the misunderstanding that machine learning techniques from one domain are not applicable to another."
- "Our field (materials science) is data sparse, we do not have a lot of data, the current excitement in AI and Digital technology is all about data. It becomes difficult to convince colleagues to join us and work with us."
- "We need to build bridges between empirical materials science data and the shiny 'data base'."
- "We have come far enough to acknowledge we need different expertise to work together. I think it is there. What is lacking is opportunity."

Theme 4. Participants appreciated the learning opportunities in meeting people from diverse backgrounds.

The enthusiasm to meet different people from parts of the ecosystem is strong across the board. The interest is beyond learning about what each other is doing and establishing research objectives; the interest extends to shifting perspectives and meeting new people as whole persons.

Below are some relevant quotes.

- "I am interested in learning about what others are doing. It has been harder since COVID because we have not had conferences."
- "I would like to find potential collaborators."
- "Talking with people from different backgrounds brings new information, and ways of thinking. I also enjoy meeting new friends and learning about them personally."

Jargons and Their Definitions

One common challenge we identified through interviews was language. As one interviewee pointed out, "sometimes we use the same language, but mean different things". So, we invited our interviewees and all our workshop participants to list "relevant yet ambiguous" terms in translational materials and give their definitions from their expertise. Some definitions are in the form of questioning. A table of some of the jargon identified from the interviews and workshop is included in Appendix 3.

Summary of themes explored:

Over 120 different initial theme ideas were identified by the workshop participants. These could be grouped into some common categories: data, applications/materials, teaming, education, policy, ecosystem, methods/tools, and funding. In the applications/materials area, topics included additive manufacturing, lossless waveguides, bio-produced recyclable polymers, plastics recycling, polymer sustainability, biopharmaceuticals, high entropy alloys, packaging materials, and anisotropic materials.

Connections to other initiatives:

As noted above this workshop built on two prior Convergence Accelerator workshops: "Design for a Circular Economy from Molecules to the Built Environment", PI M. Bilec and "Socioresilient Infrastructure: Precision Materials, Assemblages, and Systems", PI C. Ortiz. Two of the co-organizers of the former workshop, Prof. Melissa Bilec, and Prof. Gemma Jiang, were part of the organizing committee for this workshop and ensured that some of the themes and participants from their prior workshop were also involved in the current work. The molecular focus of the present workshop provides an opportunity to extend the findings of those prior workshops into a broad-based, convergent program in areas like sustainable materials or the built environment.

Another key foundation of this workshop was the long-term historical investment across multiple agencies in the Materials Genome Initiative (MGI)[5]. This investment has developed a cohort of researchers and technologies ready to accelerate materials innovation. Dr. James Warren, one of the workshop co-organizers, is a key leader in the MGI. This workshop offered a different perspective from the MGI with its explicit focus on translation and the movement of basic science discoveries to social impact.

Additionally, this workshop was explicit in its intent to connect fundamental materials science to the practical world of manufacturing. There were participants from startups, established materials companies, and large multinationals. In addition, we connected these two worlds by taking a virtual "field trip" at the end of our first workshop session to a panel discussion at a concurrent NSF Manufacturing Institute workshop. The topic of the panel discussion was the NSF Convergence Accelerator program, but it served as a forum to advertise our workshop, and three new participants with manufacturing backgrounds joined after the panel discussion. The Manufacturing USA institutes[6] offer a potential mechanism to drive further collaboration between basic research and industrial use.

Finally, a conscious effort was made to include participants from both PUI and NSF EPSCOR institutions. Interestingly, one of the themes that emerged from the discussion was the need to reduce the "barriers to sharing" that keep industry from being able to quickly identify, define, and suggest potential projects for undergraduate or master's research topics.

While the 2019 NSF "Frontiers of Materials Research: A Decadal Survey"[7] provides useful context, it largely reiterates existing efforts and themes in materials science research and fails to capture the challenges in moving materials innovation from the lab to society. It is interesting to note, however, that the challenge of sustainable polymer materials is called out explicitly in the report and was a key area of discussion for participants in the workshop.

The future of sustainable polymer materials was recently explored in the NSF "Sustainable Materials and Manufacturing Virtual Square Table"[8] sponsored by the Center for Sustainable Polymers[9] and the University of Chicago. Several participants were common between the two workshops, highlighting the important synergy between the basic science explored by the NSF Division of Materials Research (DMR) and the translational work discussed here.

In terms of cross-agency collaboration, the workshop included a variety of participants from NSF, NIST, DoD (ONR, AFRL, NRL) and DoE (Sandia).

Detailed recommendations and milestones from each theme:

1. Materials Research Data Sharing Principles & Infrastructure

Materials data is scattered and scientists are often time limited; both mean leaving data from which knowledge can be generated on the table. Although there has been much progress in this direction, we need (1) collaborative platforms, (2) dedicated support staff, and (3) shared codes for automation.

1. Collaborative platform: FAIR, open, interoperable, democratized, federates/shares materials data and metadata, enables searching, attribution, communication features (a la issues in GitHub), and IP protections (a la private repositories)
2. Data librarian (archivist): provide best practices and training in data literacy, sample solutions, long-term data management, specialized skills and expertise, save time for materials scientists
3. Shared codes for automation: open-source codes for automating simulations and experiments, parsing results, and structuring them in digital database formats; common and shared laboratory information management systems

The overall goal is to develop a plan for treating raw data not as proprietary, but as a democratized resource with proprietary interpretations. Focusing on early adopters before expanding to broader groups. Centralizing an Electronic Lab Notebook or Laboratory Information Management System between universities to allow querying between labs. Private vs. public entries for IP control. Something like Github for raw materials data.

2. Incentives for Long-term Investment & Sustainability

Incentives have to be designed to address all stakeholders (academia, government laboratories, industry, …) to work together for convergence, both at the individual and organizational level. This will require a huge cultural change. A convergence program should prototype the following incentives within the 3 year time frame

- *Rewarding data contribution* on all levels: Moving away from today's one-dimensional academic citation metrics, contributions have to be made transparent and rewarded accordingly. High quality data entries into databases are tracked and data sharing incentivized by a novel metrics, e.g. tracking (re)use of data in a database or blockchain. MS: Concept and pilot application developed based on "research use case" in the project, stakeholder feedback collected and roadmap for further implementation drafted
- Thinking big, that should include *mechanisms for protecting proprietary attributes of data* (to incentivize industry to participate) *as well a licensing mechanisms to generate long-term value*

streams for data contributors, while providing full transparency about the licensing cost for later data users in implementation. This could be implemented on a blockchain. MS: White paper developed, MVP demonstrator application with structured feedback from all stakeholders.

- Related, *novel schemes for handling IP* are needed to balance openness, inclusion of many convergence participants, while allowing attractive paths for (often desired exclusive) use by industry for scaling. A neutral holder of IP, i.e. NSF at a national level, together with clear assignments of applications fields and conditions (i.e., exclusive licenses phase out if no scaling efforts at partners) ensures maximizing technology use. MS: Scenario planning, workshop with stakeholders within and beyond accelerator program. Decision on steps towards implementation (task force).
- *Funding levels / quota in future programs depend on track record* in previous convergence programs. MS: Concept developed, Proposal for future programs drafted
- *Require convergence experience building on the personal level*: Industrial sabbatical for academic researchers, embedding of industrial researchers in project team at national lab or academic institution, internships for students in industry or at national laboratories. Dedicated funding for these formats, required to be set aside in any convergence project. MS: Case study of different embedding modes completed during the 3 year convergence program. (This would be a meta-study on the novel convergence "embedding" mechanisms on organizational and individual level (conducted during convergence program by integrated social science / management science team). Learnings and recommendations published in peer-reviewed high impact journal.

3. Full-lifecycle and Sustainability "Systems Thinking" in Materials Design

Incorporating life cycle metrics and systems thinking into the design of novel materials and processes can illuminate paths to more sustainable and scalable processes. Incorporation of these objectives would fundamentally change the way we invent materials. Historically, avoidance of these metrics has led to undesirable environmental, social, and economic outcomes.
A key barrier to routine lifecycle analysis is the scarcity of experts in the field and the cost of the process, driven by the expense of underlying databases. Key needs include:

- A program (i.e. funding mechanism) to support holistic materials discovery research that goes beyond the materials space and that incorporates more interdisciplinary perspectives that go beyond materials science (e.g socio-economics, policy, environmental issues, etc.).
- An educational transformation: students need to be encouraged to incorporate systems thinking. However, we must not dilute their disciplinary expertise. We must (a) train them to be able to appreciate and incorporate systems metrics and (b) raise a new crop of technicians who specialize in the use of these anticipatory life cycle/systems assessment tools (esp. for more sustainable materials innovation).

4. Construction of Inclusive, Large-scale Partner Ecosystems

Teams must include researchers from academia and industry, as well as experts in life cycle analysis, the biological effects of the new technology and its manufacture (i.e., cell biologists, ecologists, environmental engineers as relevant), and community outreach. Such teams are essential for accelerating the conversion of fundamental science breakthroughs to useful products that will benefit society, while also avoiding the harms from unintended consequences. A more inclusive, diverse partnership ecosystem that rallies around important global challenges could showcase materials innovation as a force for good, while also attracting socially conscious and ambitious students to the materials sciences and creating a strong pipeline at universities of people with cross-functional skills.

Creating these ecosystems requires agreement (and likely new approaches) as to how intellectual property will be handled. Embedded exchange between partner institutions will create stronger ecosystems.

Here are some ideas for milestones:

- Scoping the global challenge(s) that the partnership will address through materials R&D
- Identify key bottlenecks and address them through the creation of task groups along the TRLs but with due consideration of environmental impacts and sustainability
- Generating roadmaps & research priorities
- Ongoing pilot efforts in addressing these challenges through this partner ecosystem (fail fast?)

5. Making Materials Knowledge Consumable in Design and Manufacturing

Smarter manufacturing is the future of national economic security and resiliency. On a global scale, the next industrial and economic powerhouse will be the country or region that masters smarter manufacturing first. Manufacturing USA Institutes are putting the US in a position to do that through technology and talent development, bridging the gap in manufacturing innovation. Through support from the DOC, DOD, and DOE, the 16 Manufacturing USA Institutes link thousands of small manufacturers, two-thirds of Fortune 50 US manufacturers, and nearly every top-ranked research and engineering university in the country, accelerating the translation of use-inspired research to commercial impact. These institutes span all manufacturing sectors and share a common material data repository called the Material Commons, which democratizes data access amongst the membership ecosystem.
NSF funded programs should leverage the Manufacturing USA Institutes to bridge the gap between research and the needs of manufacturing organizations. This may be accomplished in part by:

- Continued participation of Manufacturing USA Institutes in NSF Convergence Accelerator workshops;
- Requiring inclusion of at least one Manufacturing USA institute on project teams in an advisory, technical, or workforce development capacity during Convergence Research Phase 1, Phase 2, or both project phases, as appropriate;
- Granting project teams access to the Manufacturing USA Material Commons;
- Upon project completion, require teams to upload project data to the Material Commons to expand this resource for future funded programs;
- Collaboration between Manufacturing USA and the NSF to expand the Material Commons to support expanded capability and capacity.

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References

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[4] NSF # CMMI-1940680, PI S. Min
[5] https://www.mgi.gov/
[6] https://www.manufacturingusa.com/institutes
[7] https://www.nap.edu/catalog/25244/frontiers-of-materials-research-a-decadal-survey
[8] NSF # DMR-2127823, PI J. de Pablo
[9] https://csp.umn.edu/

Appendix 1: List of Participants

Organizers:

Title	Name	Affiliation
Dr.	Jed Pitera	IBM Research
Dr.	John R. Smith	IBM Research
Dr.	James Warren	NIST
Prof.	Melissa Bilec	U. Pittsburgh
Prof.	Gemma Jiang	U. Pittsburgh

Participants:

Title	Name	Affiliation
Prof.	Ahmed Busnaina	Northeastern
Prof.	Ale Strachan	Purdue
Dr.	Alysia Garmulewicz	Materiom
Dr.	Amberlee Haselhuhn	LIFT
Prof.	Amy Peterson	U Mass Lowell
Dr.	Anne Fischer	DARPA
Dr.	Bernhard von Vacano	BASF
Dr.	Bob Bartolo	N/A
Dr.	Bryan Boudouris	NSF
Prof.	Chris Hansen	U Mass Lowell
Dr.	Christina Baker	PPG
Dr.	Damon A. Dozier	MRS
Dr.	Dave Rejeski	N/A
Dr.	David Furrer	Pratt & Whitney
Dr.	Debra Audus	NIST
Prof.	Desiree Plata	MIT
Prof.	Emmanuel Arzuaga	U Puerto Rico
Dr.	Eric Lin	NIST
Ms.	Erika Strassburger	Pittsburgh City Council
Dr.	George Spanos	TMS
Mr.	Gregory Dreicer	N/A
Prof.	Huimin Zhao	UIUC
Mr.	Ian Garretson	UC Davis
Mr.	Jeffrey Buenaflor	U Minnesota

Prof.	Jin Wen	Drexel
Dr.	John Schlueter	NSF
Dr.	Julie Christodoulou	US ONR
Dr.	Kate Beers	NIST
Prof.	Kristofer Reyes	U Buffalo
Prof.	Lav Varshney	UIUC
Prof.	Lawrence Hill	Western Kentucky U
Dr.	Linda Molnar	NSF
Dr.	Linda Sapochak	NSF
Prof.	Manuel Rodriguez	U Puerto Rico
Prof.	Mark Asta	UC Berkeley
Dr.	Max Teplitski	Produce Marketing Association
Prof.	Michael Cai Wang	U South Florida
Dr.	Michael Durstock	US AFRL
Dr.	Molly Morse	Mango Materials
Ms.	Nina Jankovic	Yale
Dr.	Nora Savage - NSF	NSF
Dr.	Patrick Fuller	NuMat
Prof.	Peter Voorhees	Northwestern
Prof.	Prasanna Balachandran	U Virginia
Prof.	Raymundo Arroyave	Texas A & M
Prof.	Rodney Andrews	U Kentucky
Dr.	Sarah Topper	PPG
Prof.	Thomas O'Connor	Sandia National Labs / CMU
Dr.	Yibin XU	NIMS (Japan)
Dr.	Brian Decost	NIST
Dr.	Elizabeth Ryland	US NRL

Appendix 2: Detailed workshop agenda

Watch Party/Tech Support, May 17

5 min: KI introduction, review agenda
5 min: Welcome from organizers
5 min: Introduction to KIStorm virtual event space
15 min: Pre-recorded video from Prof. Melissa Bilec (Pitt) on lessons learned from prior Convergence Accelerator Workshops
15 min: Pre-recorded video from Dr. Linda Molnar (NSF) and Dr. Linda Sapochak (NSF) on the details of the Convergence Accelerator program
10 min: Quick small-group breakout sessions for introductions, talking about “global challenges that materials might address”
15 min: Pre-recorded video from Dr. Anne Fischer (DARPA) discussing challenges and opportunities in materials innovation and automation.

10 min: Second small-group breakout session for introductions, talking about "potential materials and supply chain innovations"
5 min: Closing and steps for next session

Session 1, May 20

Recorded pre-work: Discussion with Dr. James Warren (NIST) and Prof. Alan Aspuru-Guzik (U. Toronto) on the current state of Materials Discovery
5 min: KI Introduction, review agenda
10 min: Welcome from organizers (Jed/John)
10 min: Review of Convergence Accelerator objectives (Linda Molnar)
5 min: Overview of KIStorm platform, mechanisms for collecting ideas
40 min: 3 rounds of small group breakout networking

- Round 1: If we could change one thing about the way we discover/develop new materials, it would be.....
- Round 2: If we were to proudly present a "translational materials" solution together in 5 years time - what would the title be.... and What did you have to overcome to get you here
- Round 3: What are the impediments or weak links in our materials discovery/development ecosystem?

40 min: Panel Q&A discussion
15 min: Break
5 min: Welcome back/reset
35 min: Small breakout groups to identify challenges, posted on KIStorm

- What is it that blocks the intersection of materials discovery and advanced manufacturing? - Why doesn't the current practice of materials discovery include all voices, perspectives, and stakeholders?
- What's stopping us from building "communities of discovery" that are more effective for scale and impact?

10 min: Closing statements
Transition to NSF Manufacturing Workshop Panel (https://pwd.aa.ufl.edu/nsf-advmfgworkshop/)

Session 2, May 24

Recorded pre-work: Description of the NSF MMLI center from Prof. Huimin Zhao (UIUC), dialogue on materials innovation between Ms. Nina Jankovic (Yale) and Prof Desiree Plata (MIT)
5 min: Welcome back/reset
15 min: Discussion of community challenges selected for further discussion – the "Spicy Wall"
25 min: Small breakout groups

- 1) How might we make better decisions about global-scale materials investments?
- 2) Take a look at the "Spicy Wall" of filtered topics -- what's missing? What needs to be added?

20 min: Break and vote on topics with 5 votes/person
10 min: Select top 5 challenges and promote to discussion topics, ask people to sign up
55 min: Breakout to discussion topics, fill in initial template for each topic

10 min: Break
5 min: Welcome back
30 min: Readouts from each discussion group
5 min: Closing statements, reminder for next session

Session 3, June 1
Recorded pre-work: Discussions on materials innovation and translation to industry from Prof. Peter Voorhees (Northwestern) and Dr. Bernhard Ulrich von Vacano (BASF)
25 min: Review of Convergence Accelerator goals and revised topic template (Linda Molnar, Jed Pitera)
60 min: Breakout to discussion topics, complete Session 2 template and new Session 3 prompts
20 min: Break
40 min: Readouts from each discussion group
20 min: Full-group discussion and feedback
15 min: Acknowledgements, thanks & closing comments

Appendix 3: The "Jargon Wall" – working toward a common language

Term	**Expertise**	**Definition**
AI	Computational material	Using computers algorithms to reason about environments, person and actions, and get some fundamental understanding of the system
Automation	Computational material	Integration of robotics, to perform manufacturing, or materials research; Autonomy: robotics can think for themselves
Autonomous lab	Industry	What degree of autonomy, just machine learning, or also includes machine reasoning incorporating AI?
Branding	Industry	Branding a material so it can tell a story
Creativity	Computational material	Generation and selection of ideas and artifacts that are both novel and judged to be high quality by experts in the field.
Data/Cyber infrastructure	Computational material	Combination of tools to facilitate the storage, moving and retrieval of data
Design	Material science	Given many possibilities, what would be an ideal recipe to explore next
Design for end of life	Industry	Where is the polymer/material going to end up--recycled? composed? biodegraded?
Digital twin	Mathematician	Usually used in industrial products to refer to a digital artifact (think database) that captures all of the design, manufacturing, use, and repair details of a complex product like a jet engine. Anything that happens to the first (real) twin gets recorded in the digital twin. This captures important history but also allows the creation of models for reliability, predictive maintenance, etc.
Emulator	Mathematician	Computational model that captures the precise evolution of a system with little or no uncertainty, such that it is equivalent to the original system; a modern computer can easily run an Apple II emulator.

Impact	Computational material	Scientific, societal, internal (fun, curiosity)
Machine learning	Computational material	A subset of AI using statistical models
Material discovery	Business	Profitable materials
	Data scientist	Data driven
	Material scientist	Fundamental research
Policy	Material science	A specific question that we are trying to pose in order to define where the design should be. A policy should help us make the decisions given the context; it has a theoretical and mathematical foundation. Policy helps you make informed decisions on design.
Proof of concept	Academic	Experiment that shows it is not impossible; it is publishable
	Industry	Something that shows it is feasible and viable, shows the path that is it scalable and profitable
Robust model	Material science	How much data we need to create robust models. While that thought encompasses a thriving area of research, it can be useful to make sure that people are aligning their data science approaches to the limitations of the experiments/simulations that the training datasets are derived from (or develop new experimental/simulation strategies to overcome those limitations).
Simulator	Mathematician	An approximate model of a system, usually based in fundamental physics/chemistry, that can have uncertainty because of statistics, approximations, or incomplete details.
Data sparsity	Material science	lack of data, small data, missing data
Surrogate model	Mathematician	This is a broad term, but in general in a AI/ML context it refers to a model that predicts difficult- or expensive-to-measure properties from more easily observed ones. For example, a model that can predict the expected lifetime of a component in years based on observations from the first few weeks of use. Often used in materials to refer to models that take "cheap" simulation inputs and correct them to accurately predict "expensive" real-world properties.
Translational materials	Computational material	How do we deliver actual tangible results from material lab discovery to real world use
Uncertainty	Material science	What you do not know, very difficult to pinpoint that source of uncertainty. It could result from lack of knowledge (material scientists believe it could come from lack of physics, so we need to account for the principles) or lack of data (data driven approaches believe everything is in the data)

Use inspired research	Industry	design with an end in mind

Appendix 4: Working documents from working groups 1-5

Group 1:

Title: Materials Data Sharing & Infrastructure **Laboratory Data Standardization and Failure Reporting (?)**
Please write your name and email: • Patrick Fuller (pat@numat.tech) • Gemma Jiang (gemmajiang@pitt.edu) • Michael Durstock • Debra Audus (debra.audus@nist.gov) • Elizabeth Ryland (elizabeth.s.ryland@gmail.com) • Brian DeCost (brian.decost@nist.gov) •
What's the big idea (2 to 3 sentence summary)? Why is this a game changer? Materials data is scattered and scientists are often time limited both mean leaving data from which knowledge can be generated on the table. Although there have been much progress in this direction, we need (1) collaborative platforms, (2) dedicated support staff, (3) shared custom codes for automation 1. Collaborative platform requirements: interoperable, federates materials data and metadata, enables searching, attribution, communication features (a la issues in GitHub), IP protections (a la private repositories), democratized 2. Data librarian (archivist) requirements: provide best practices, lists of solutions Develop a plan for treating raw, plain-text data not as proprietary, but as a democratized resource with proprietary interpretations. Focusing on early adopters before expanding to broader groups. Centralizing an Electronic Lab Notebook or Laboratory Information Management System between universities to allow querying between labs. Private vs. public entries for IP control. Github for raw materials data. • How do we add data tagging (provenance), curation, and centralize submission?

- How do we open up IP-centric companies and controlled government data (CUI)?
- Culture - academic subgroups (e.g. bioinformatics vs. cheminformatics) and their tendency to share. Synthetic/organic groups - very competitive, secretive, won't be open to sharing. IP-focused companies - not open to sharing, prefer walled gardens.
- Distinguishing features of closed vs open communities.
- Why does the current system exist?
    - Academia - hold on to hard-to-generate data until can publish
    - Industry - IP issues, sharing from business perspective to create sticky customers (walled gardens, vendor lock-in)
- Missing infrastructure
    - Has to be easy, otherwise will not adopt over existing workflows
    - Cannot require coding skills - synthetic labs do not have capability
    - Needs to be flexible and interoperable (open data formats prioritized over strict standardization; interface control documents)
- How do you sell ELN / data to academia/industry
    - Funding / prestige
    - Safety is a strong sell for ELN; can we get multi-university adoption?
- Need other data, too (environmental, safety, cost, impacts)
- How to motivate contributing rather than lurking
- Needs to be a generic platform to spur broader usage.
- Private sections (a la GitHub)

Who needs to be involved in the discussion on this topic (implementers, stakeholders, educators, etc.)?

Provide the "how" of data information management: Library scientists, data scientists (from economics, bioinformatics, and other big-data industries), Journals/publishing: Elsivier, AIP, etc.

Provide the "what" and "why": industry R&D, academia, manufacturing

What are the anticipated transformative *__societal__* and *__scientific__* impacts? What will be disruptive? THINK BIG.

- Data manager in each lab(/department/university); the new era of librarians
    - NSF actively funding library scientists/ students in labs
- Shared system / plain text data sharing between universities
    - NSF actively funding open ELN implementations
    - NSF actively funding research collaborations: funded "partnered papers" analytical/data interpretations of "communal" data from a partnered data-generators
- Training
    - NSF-funded workshops for AI/ML

Direct impacts over the next 3 years:

- Papers based on communal data for accelerated discovery
- Expand the data available into resource-deficit communities

Subsequent impacts over next 10 years:

- Papers based on others data for accelerated discovery / access to broader talent pool / democratization of science
- Drastically increase the

What are the barriers preventing this from happening right now?

- Why does the current system exist?
    - Academia - hold on to hard-to-generate data until can publish
    - Industry - IP issues, sharing from business perspective to create sticky customers (walled gardens, vendor lock-in)

What is needed to get us started?

What might be all the products, proof of concepts, prototypes, you can think of?

What are major milestones? How will we know we are "on track"?

For the remaining questions, imagine that you are all part of a Convergence Accelerator team funded by NSF to address one of the barriers or lead to one of the impacts above. You have three years of significant funding to make a difference.

What does your team composition look like? What kind of skills, backgrounds, expertise are involved?

- Data archivists
    - https://link.springer.com/article/10.1007/s10502-020-09330-3
    - https://core.ac.uk/download/pdf/223094159.pdf
- Data scientists
- Material scientists
- Statisticians/experts in mathematical analysis of large data
- Decentralized team (1x/institution) who report to central project manager matrixed with dept/lab PI
- Industry/manufacturing partners

What are three measurable results your team is working towards? It may help to use the SMART framework -- goals should be Specific, Measurable, Attainable, Relevant and Time-Based.

6 month goal:
NSF-funded workshops for learning AI/ML

data archivists hired at numerous institutions (R1, govt, PUI, community colleges, industry etc.)

1.5 year goal:
Getting data into the hands of those in need:
- several prototypes for how different types of data from different institutions can be shared
- hold a round robin for data analysis
- "white papers" for projects/publications on open-source analysis of raw data
- incentivization structure for open data (for industry): greater talent pool

3 year goal:
- publications that use data from other institutions
- connections to industry
- initiated collaborations between multiple institutions
- a functional multi-institution example of using of a data archival system

How does the technical and organizational diversity of the team improve your ability to achieve these goals? In other words, why is this a Convergence project?
Bringing together input from multiple disciplines (data generators, data analysts) and industries, scientific publishing etc. is necessary to solve this sort of joint problem.

The goal of this initiative is to make raw data files interoperable and collaborative interpretation, thus it is necessary that this is a multiple institution venture. This initiative will draw on the knowledge of data statisticians, analysts, archivists to organize and make interoperable the vast materials data held in distinct institutions.

How would this team's work connect to or leverage other initiatives or programs? Examples include other NSF programs, other funding agencies or governmental organizations, or non-profit or international efforts.

Convergence accelerator Track D: AI-Driven Innovation via Data and Model Sharing
Materials Genome Initiative
DMREF
MURI

Projects:
- Materials Project
- Materials Data Facility
- DataHub
- AllTrials
- ...

Please be prepared to give a 3-minute summary for the group. We will hear summaries from each group when we reconvene in the plenary.

(we will screen share your document and give you an indication of 30 seconds time remaining)

Group 2:

Title: How might we create specific incentives for people, or organizations, to invest the time and effort, especially over a reasonably long time horizon, to learn from and collaborate with the many stakeholders? **How do we incentivize capital flow into a circular economy, where products end up back where somebody can reuse/reprocess them? Can we convert these circular materials/products into investible tokens?**
Please write your name and email: • George Spanos (TMS) gspanos@tms.org • Molly Morse (Mango Materials) Molly@MangoMaterials.com • Bernhard von Vacano (BASF) bernhard.von-vacano@basf.com • Linda Molnar (NSF) • Christina Baker (PPG) CBaker@ppg.com • Lawrence Hill (Western Kentucky University) lawrence.hill@wku.edu
What's the big idea (2 to 3 sentence summary)? Why is this a game changer? We must find ways to incentivize stakeholders from academia, government laboratories, and industry to work together in a collaborative/convergence way. The incentives have to be at both the individual level and the organizational level. It must be both a top down (e.g., funding agencies, high level managers) and bottoms up (individual researchers/engineers) approach, and will involve a huge cultural change.
Who needs to be involved in the discussion on this topic (implementers, stakeholders, educators, etc.)? **Gov. funding agencies/NSF** - the funding "stick" **Industry** - must get them involved in the early stages well before the valley of death - what incentivizes these individuals? Pre Competitive space - push that line as far as we can. First define where it is now, then how far can we go in the convergence realm. Academic licensing structure, carve out different potential applications fields early? **Academia** - early stage - professors doing fundamental stage research (but without squelching their creativity/innovation). **Government laboratories** - they are answerable to their ultimate clients (e.g. the warfighter, public taxpayer, etc.)

What are the anticipated transformative *societal* and *scientific* impacts? What will be disruptive? THINK BIG.

Direct impacts over the next 3 years:

A product/component that has passed through (or avoided) the valley of death

In addition to technical achievement, a package of validated deliverables for a convergence project, including

- LCA / sensitivity analysis
- (Rough) concepts/scenarios for manufacturability
- Most promising fields for commercialization
- A map of continued and new partners needed to support the next steps
- ...

Partner early career professionals with large companies for development of new materials and products

Measureable handoff between research and corporate environment could also include talent trained on relevant methods and in relevant domain, in addition to traditional deliverables (IP, prototype, …)

Subsequent impacts over next 10 years:

Create long term interconnected networks between researchers and commercial partners

NSF is an ideal neutral party and could hold the patents and technology that is developed through early stage research and corporate investments. Large companies could have potentially limited scopes or fields allowing the research to be used further elsewhere, or to have a life if the large company decides not to outright buy, or further invent in the commercialization.

What are the barriers preventing this from happening right now?

Companies want to gain the value of their investment
The time it takes for early stage development

What is needed to get us started?
A kickoff meeting that brings together an interdisciplinary group of stakeholders from academia, government, and industry that does a deep dive to begin going back to their organizations to begin implementing the specific recommendations developed at this convergence workshop, into their individual home organizations.

Discrete survey(s) of key industry stakeholders to gain more detailed knowledge of the implementability of the suggested incentivization methodologies into their organizations

A funding scheme that supports (and requires) all required capabilities to be included in the team, with a time horizon and commitment that matches the timeline and scale of a given challenge (ideally to be defined as an end-to-end innovation process)

What might be all the products, proof of concepts, prototypes, you can think of?
A few new materials discovery, development, and deployment accelerator networks

Detailed, transferable learnings from following a convergence research project and documenting decisions, reasoning and outcomes at different stages and phases: E.g. from embedded team of social scientists / management science group.

What are major milestones? How will we know we are "on track"?
Life Cycle Analysis (LCA)
The number of new innovations or materials resulting from these networks

For the remaining questions, imagine that you are all part of a Convergence Accelerator team funded by NSF to address one of the barriers or lead to one of the impacts above. You have three years of significant funding to make a difference.

What does your team composition look like? What kind of skills, backgrounds, expertise are involved?

Researchers and engineers from industry, national laboratories, and academia across disciplines including materials science and engineering, data science, chemistry, designers, environmental scientists, agile manufacturing experts

Business/commercialization experts, social scientists (e.g., for cultural barriers)

What are three measurable results your team is working towards? It may help to use the SMART framework -- goals should be Specific, Measurable, Attainable, Relevant and Time-Based.

Overarching comment: Develop a new materials/manufacturing innovation over the product development cycle from discovery of a new material or materials process, to development, toward commercial product deployment

6 month goal:
○ Training/Hand-off early on for development to train academic partners on the industrial needs - any format (workshops, meetings, etc.)
○ Scope out the lifecycle of a new materials/manufacturing innovation from the beginning - include as a starting deliverable.
○ Identify gaps in data and unknowns, strategy to fill and acquire data
○ Agile project management training to assist with nimbleness of projects and complexity of multiple institutions development - hire a dedicated person? Establish tool like Trello?
○ Data / automation concept

1.5 year goal:
○ Industrial sabbatical for academic researchers, embedding of industrial researchers in project team at national lab or academic institution
○ Internships for students in industry or at national laboratories, working on the new materials/manufacturing innovation
○ Bringing early career corporate professionals into academic environment
○ Presentations, publications and citations of proof of concept of prioritized materials or manufacturing process

3 year goal:
○ Researchers versed and trained in materials manufacturing, scaling and commercialization aspects, beyond individual postdoc
○ Patents, publications
○ Trained employees for industry
○ Corporate partnerships
○ IP agreements
○ Prototype with manufacturability concept, LCA, understanding of remaining uncertainties…
○ FAIR data repository

How does the technical and organizational diversity of the team improve your ability to achieve these goals? In other words, why is this a Convergence project?

Inclusion of interdisciplinary technical capabilities, augmented with other stakeholders (e.g. for sustainability considerations, regulatory, social impact), training and education as integral component, automation and digital sciences, "meta-level" analysis of project mechanics to identify success factors and learnings to develop blueprints for future convergence projects.

How would this team's work connect to or leverage other initiatives or programs? Examples include other NSF programs, other funding agencies or governmental organizations, or non-profit or international efforts.

NSF ERCs where applicable if technical overlap

DoD or DoE Centers of Excellence and/or national laboratories where appropriate leveraging

Manufacturing USA Institutes (America Makes)

Joint funding, project handover for commercialization or implementation (e.g. With DoD)

How to interact: Joint meetings, symposia, publications, and funding proposals/awards

Please be prepared to give a 3-minute summary for the group. We will hear summaries from each group when we reconvene in the plenary.

(we will screen share your document and give you an indication of 30 seconds time remaining)

Group 3:

Title: A lifecycle tool for systems thinking
Please write your name and email: • Raymundo Arróyave, rarroyave@tamu.edu • Desree Plata, dplata@mit.edu • Gregory Dreicer gdreicer@gmail.com • Alysia Garmulewiez, alysia@materiom.org • Kristofer Reyes, kreyes3@buffalo.edu Day 3: Added • Ahmed Busnaina; busnaina@coe.neu.edu • Dave Rejeski; rejeski@eli.org
What's the big idea (2 to 3 sentence summary)? Why is this a game changer? Incorporating life cycle metrics and systems thinking into the design of novel materials and processes can illuminate paths to more sustainable and scalable processes. Incorporation of these objectives would fundamentally change the way we invent materials. Historically, avoidance of these metrics has led to undesirable environmental, social, and economic outcomes.
Who needs to be involved in the discussion on this topic (implementers, stakeholders, educators, etc.)? Social scientists and historians Engineers (e.g., materials, environmental, chemical) Political scientists Computer scientists Governments Educational Institutions/ Educators
What are the anticipated transformative *<u>societal</u>* and *<u>scientific</u>* impacts? What will be disruptive? THINK BIG. **Direct impacts over the next 3 years:** We are very far away from having the ability to access life cycle implications in a streamlined way that can inform design and development of novel materials and processes. However, the methodology and workflows for these assessments can be simplified and shared in a way to reduce costs, acknowledge uncertainties, and expand the application of transdisciplinary,

systems assessments. This needs to be constructed, so the immediate 3-year impacts would be mobilization of communities of researchers to answer basic questions, such as:
-what are the minimum criteria needed to understand environmental fate?
-how can and should one assess social impacts locally? Engage community members in design and implementation of technology and processing?
-how do we understand or quantify uncertainty in data-sparse fields? What is the minimum amount we need to know to avoid being completely wrong?
-how do we assess cost and supply chain implications in real time?
-what can we learn from historical examples, community stories, and costs (e.g., when systems thinking wasn't incorporated proactively).
-how do we leverage datasets of varying scales? How do we encourage dynamic data repositories?

Subsequent impacts over next 10 years:

Improved incorporation of systems impacts into the design process such that cost and unwanted social/environmental impacts can be avoided *while* materials performance and profits are maximized.

What are the barriers preventing this from happening right now?

It is computationally complex (life cycle assessment) and the data are missing with respect to novel materials. Because systems assessment across the life cycle is difficult and costly, it is often not done until a process is scaled (when it might be too late to inform decision making). We need to (a) streamline life cycle assessment, (b) leverage existing data, and (c) add/incorporate/encourage social impact assessment.

The data that do exist are behind paywalls, so they are functionally inaccessible to "start ups" and students. (and large companies are not motivated to purchase these).

ISO standards are remarkably strict. These could be prohibitive to innovation and recognition of alternative pathways.

What is needed to get us started?

A program (i.e. funding mechanism) to support holistic materials discovery research that goes beyond the materials space and that incorporates more interdisciplinary perspectives that go beyond materials science (e.g socio-economics, policy, environmental issues, etc.).
And also an educational transformation: students need to be encouraged to incorporate systems thinking. However, we musn't dilute their disciplinary expertise. We must (a) train them to be able to appreciate and incorporate systems metrics and (b) raise a new crop of technicians who specialize in the use of these anticipatory life cycle/systems assessment tools (esp. for more sustainable materials innovation).

What might be all the products, proof of concepts, prototypes, you can think of?

Ashby-like Materials Selection Tools that Incorporate Life Cycle-Relevant Metrics
EcoImpact tools + other LCA tools

We seek to encourage an open data model that supports uncertainty and sparse data. This could be quantified for user transparency.

A data schema for measurement of systemic impacts could be developed using schema.org to encourage collective development and general adherence to FAIR data principles

What are major milestones? How will we know we are "on track"?

A great mid-point success would be the establishment of an open-data repository and workflow (with a GUI) that is both usable but also encourages uploading and curation of data.

Here, we note that improvements in machine-readable publications will accelerate the collection of this type of information in a way that supports faster, higher throughput assessment of impact and life cycle considerations in a way that enables one to incorporate these assessments into the innovation/decision making process.

For the remaining questions, imagine that you are all part of a Convergence Accelerator team funded by NSF to address one of the barriers or lead to one of the impacts above. You have three years of significant funding to make a difference.

What does your team composition look like? What kind of skills, backgrounds, expertise are involved?

- Materials/Chemists/Physicists
- Manufacturing
- OR/IE
- AI/ML
- Environmental Scientists, Ecologists
- Problem/Application owners/stakeholders, industrial partners
- Lawyers, Political scientists, Historians, Sociologists
- Facilitators, project management, communicators

What are three measurable results your team is working towards? It may help to use the SMART framework -- goals should be Specific, Measurable, Attainable, Relevant and Time-Based.

6 month goal:
- Review precedent (lessons learned)
- Develop guidelines for process, including goal-setting, organization of heterogeneous set of stakeholders
- Stand-up data repository, define data policies

- Coordination of research activities between different fields

1.5 year goal:

- Prototype (sustainable) digital twin for materials design and downstream processes
- Initial population of sustainable materials for applications for review for reviewers / investors / funding agencies
- Technical courses for cross-collaboration (i.e. preserve disciplinary expertise while enabling cross-talk between the disciplines)

3 year goal:

- Application of established processes to specific projects, other parts of convergence accelerator.

How does the technical and organizational diversity of the team improve your ability to achieve these goals? In other words, why is this a Convergence project?

Broadly speaking, the problem is inherently convergent because it requires transdisciplinary integration and coordination of research. In order to achieve multi-objective materials optimization (e.g., social, economic, environmental, and materials performance impacts), all stakeholders need to be engaged in the research process. (For example, fundamental understanding of what gives rise to material performance and fundamental understanding of what gives rise to material toxicity can only inform future design if the same set of materials are tested).

Of particular importance is that materials companies or industries should be present to inform most-urgent research needs as well as the guidelines that are being developed. They should also help guide the development of trainees in a way that will both help achieve the technical objectives as well as cross train students to understand "sustainable innovation" tools that might emerge.

Including policy experts and architects is critical to build incentivization structures for investments that can help carry technology to the development scale. [This might address the question below].

How would this team's work connect to or leverage other initiatives or programs? Examples include other NSF programs, other funding agencies or governmental organizations, or non-profit or international efforts.

Specifically: NIEHS, USDA, USGS are natural partners. (Bruce Hamilton's Sustainability program would be a great add really too). There are very few not for profits that engage in the materials discovery space, but it is possible that some pro-social or environmental organizations could be engaged to help with community organization efforts and or job creation/training initiatives that are relevant to corporations who are affected by materials sustainability challenges.

Other considerations:
This is beyond the scope of the NSF, but one thing to consider in the "valley of death" is that investors are disincentivized from investing in transformative technologies. This is associated with the long return on investment timeline, which promotes investment in short-term return, software based technologies. An opportunity might exist to incentivize this type of investment via tax benefits (e.g., such as conservation easements or as we do with natural gas infrastructure development). Other than moral or philanthropic motivators, there are few motivators to investing in sustainable technologies or "tough tech" problems.

Another challenge exists in the academic rewards structure. Individuals who are trained in green chemistry and engineering or life cycle assessment often have trouble landing academic jobs or securing federal grant dollars. These "more applied" research needs should be valued by academic institutions. NSF could address this by creating an NSF CAREER-level type "CONVERGENCE Award" or something along those lines. Further, tenure-track faculty need to be rewarded for having impact on real problems in the near term (and not just far future implications).

It would be good for the NSF to also push on those who negotiate the federal overhead rates to ask universities to reflect on their engagement principles with companies. Most universities are terrible at engaging in research with businesses- large or small. This discourages businesses from bringing their problems to universities.

Please be prepared to give a 3-minute summary for the group. We will hear summaries from each group when we reconvene in the plenary.

(we will screen share your document and give you an indication of 30 seconds time remaining)

Group 4:

Title: How might we create a more comprehensive, larger-scale, inclusive partnership ecosystem to capture the full spectrum of impacts of materials design

Please write your name and email:

- Sarah Topper, stopper@ppg.com.
- Jim Warren, james.warren@nist.gov
- Julie C julie.christodoulou@navy.mil
- Amy Peterson, amy_peterson@uml.edu
- John R. Smith, jsmith@us.ibm.com

What's the big idea (2 to 3 sentence summary)? Why is this a game changer?

Stakeholder alignment and cooperation (across academia, industry, labs, gov't) improves impact for materials design.

Forming cross-functional teams around specific materials challenges that additionally tackle specific barriers for collaboration will improve speed and scale for materials translation as well as create and test new models for holistic collaboration. There is a deepening appreciation of the environmental issues around materials in manufacturing that can be considered with a more holistic systems approach. A more inclusive, diverse partnership ecosystem that rallies around important global challenges could re-establish materials innovation as a force for good … with all benefits of attracting best talent (passionate and ambitious students) and creating strong pipeline at universities, etc. A flexible, dynamic environment that enables interested parties to find each other and develop partnerships to meet their needs. Create a model(s) for industrial/academic engagement in specific materials areas X; ensure models areas of interest drive opportunities for cross-functional collaboration (e.g. incorporate life cycle analysis requirements, data management/communication, etc.)
Who needs to be involved in the discussion on this topic (implementers, stakeholders, educators, etc.)? Stakeholders - participants in the ecosystem (includes educators, researchers/ developers, manufacturers, etc.) Implementers - someone to build the enabling framework for the ecosystem and create/drive incentives
What are the anticipated transformative *societal* and *scientific* impacts? What will be disruptive? THINK BIG. **Direct impacts over the next 3 years:** Students trained in materials area X have direct experience in industrial impact Industry sees translation of cutting edge academic approaches into their R&D Industry has access to researchers with relevant training **Subsequent impacts over next 10 years:** End-to-end development of materials (from basic science to manufacturing to impact) is 10x-100x faster and cheaper. Achieve better designs via the partnership ecosystem that are more effective, less problematic (good, well targeted, quality designs) Tackle significant global problems related to health, environment, social.

Uptake in student enrollment in materials.
What are the barriers preventing this from happening right now? Weak/varied incentives for social/environmental impacts of materials research (policy/job market)
What is needed to get us started? Mechanisms ("dating app") that enables potential participants to identify others and form self-directed teams where IP considerations could be manageable Better understanding of relevant incentives for full spectrum of stakeholders
What might be all the products, proof of concepts, prototypes, you can think of? Opportunity for aligning learning/training within this theme. Being effective members of inclusive and diverse teams will be important for future leaders, also something that is of interest to students. What are the skillsets that are needed?
What are major milestones? How will we know we are "on track"? Engagement from stakeholders who aren't currently participating in similar environments Quantifiably faster failure - case studies Uptake in students studying materials/mfg Visible increase in cross-functional collaboration outputs
For the remaining questions, imagine that you are all part of a Convergence Accelerator team funded by NSF to address one of the barriers or lead to one of the impacts above. You have three years of significant funding to make a difference.
What does your team composition look like? What kind of skills, backgrounds, expertise are involved? **Ideal is a more holistic cross-functional team with fundamental research, industry knowledge of scale feasibility, and customer research on needs (How do we know what to do and how to do it?). The team includes stakeholders across the end-to-end innovation supply chain.** **How do we make sure that externalities that may not be properly priced by the market are accounted for? What people are needed for this? Experts in life-cycle analysis, sustainability ; experts who can inform studies detailing impacts of materials development/mfg/use on impacted communities**
What are three measurable results your team is working towards? It may help to use the SMART framework -- goals should be Specific, Measurable, Attainable, Relevant and Time-Based.

***6 month goal*: Form initial, inclusive cross-functional team and refine and clearly delineate an agreed-upon problem statement, roles and responsibilities, accountabilities, and deliverables. Programs should identify specific barriers required for holistic research, development and deployment that will be overcome and how. This can include new approaches for technology, infrastructure, data, IP, and more.** ***1.5 year goal*: Embedded exchange of people cross-functionally; milestones incorporated to ensure externalities are being addressed and making measurable progress; Identify impacted communities, solicit feedback, and assess implications.** ***3 year goal*: Implementation of forward path for project-generated IP; explore new models of IP management?**
How does the technical and organizational diversity of the team improve your ability to achieve these goals? In other words, why is this a Convergence project? **Having diverse voices ensures that all of the social/environmental/etc. Implications of the materials development are incorporated not at the end as an afterthought, but from the beginning of the materials development.** **Having the voice of manufacturing and end users accelerates early-stage design through use-driven development. Must not allow focus on the end goal to overly constrain possible solution spaces in early development though.**
How would this team's work connect to or leverage other initiatives or programs? Examples include other NSF programs, other funding agencies or governmental organizations, or non-profit or international efforts. **Connects to the Future of Work at the Human-Technology Frontier (impacted communities)** **Arguably this connects to an enormous number of NSF programs, as it's a modality for maximum impact**
Please be prepared to give a 3-minute summary for the group. We will hear summaries from each group when we reconvene in the plenary. *(we will screen share your document and give you an indication of 30 seconds time remaining)*

Group 5:

Title: Making materials knowledge universally accessible and useful in manufacturing
Please write your name and email:

- Peter Voorhees, p-voorhees@northwestern.edu
- Amberlee Haselhuhn, ahaselhuhn@almmii.org
- Ale Strachan "strachan@purdue.edu"
- Jed Pitera, pitera@us.ibm.com
- Thomas O'Connor, thomaso@andrew.cmu.edu
- Prasanna V. Balachandran, pvb5e@virginia.edu

What's the big idea (2 to 3 sentence summary)? Why is this a game changer?

-Transform US manufacturing - bring research closer will give competitive advantage
-Bridge the valley of death by accelerating innovation from MRL/TRL 1-3 to MRL/TRL 8-10.
-Drive innovation in materials manufacturing by educating *purchasers of materials* of innovative material capabilities.

Who needs to be involved in the discussion on this topic (implementers, stakeholders, educators, etc.)?

Manufacturing industry, academia, funding organizations, manufacturing hubs/industry consortia, non-traditional education, buyers/end users

What are the anticipated transformative *societal* and *scientific* impacts? What will be disruptive? THINK BIG.

Direct impacts over the next 3 years:

-Building of a more technologically capable workforce capable of maintaining/attracting advanced manufacturing jobs/capability within the U.S.. This may be accomplished by:

- Collaboration with professional societies to extend their training camps, i.e., ASM Teachers Camps, by 1 day to include a special "Materials in Manufacturing" session
- Outreach with FIRST Robotics, Girl Scouts of America, Boy Scouts of America, and similar organizations by individuals working in Use-Inspired Research/Design & Manufacturers to increase awareness of the link between science and manufacturing innovation
- Double (triple, x10) the number of capstone design projects sponsored/motivated by manufacturing needs
- Establish re-training centers to train displaced or transitioning workers with manufacturing/technology skills critical for US infrastructure/national security. Examples: Re-training of military members close to un-enlistment or recent veterans; training of coal miners in green-energy skills
- National public service announcements on manufacturing's role in enabling "cool" technologies: Mars Rover, SpaceX, Tesla, iPad, etc. easily identifiable by general audience. Target standard media (television commercial, magazine ad) and "new" media (Facebook, TikTok, Twitter, Instagram). Potential buy-in from corporate entities for publicity.

- Enlist or train scientists and manufacturers to be “Science Influencers” or “Manufacturing Influencers” as part of their education and/or work, where allowed - opportunities here to highlight diversity in science/manufacturing and also the innovative work being done.

- Independence from other countries for manufacturing capability (national defense initiative)
- Enable co-design of materials with applications and manufacturing
- Eliminate technology constraints in manufacturing by establishing direct pipeline of innovation to commercialization, via:
  - Establish a program for that will support sabbaticals for faculty in which they spend 9 months - 1 year working at a manufacturing organization
  - Alter funding paradigm to prioritize public-private partnerships (e.g., commercial manufacturer with academic institution)
  - Coordinate with ABET or other accreditors to require inclusion of college course on technology communication

Subsequent impacts over next 10 years:

-Reduced environmental impact from manufacturing activities as they are sourced within our nation’s borders
-Enhanced collaboration between industry and academia, strengthening the open innovation model
-More agile manufacturing industry capable of withstanding disruption
- Rapid acceleration of new technology into the customer’s hands

What are the barriers preventing this from happening right now?
-Lack of interaction between manufacturing and basic research (even within an organization)
-Challenge of data sharing between fundamental research, engineering, design and manufacturing even happens within large companies.
-Manufacturing engineers are conscious of the risk associated with adopting new technologies

What is needed to get us started?

- Government support to encourage collaboration between all of the players
- Funding (from US Government, manufacturers, etc.) to establish new programs/extend current programs
- People: Boots on the ground to drive this
- Creation of jobs within funding agencies, manufacturing organizations to lead outreach efforts and oversight of early-career sabbaticals

What might be all the products, proof of concepts, prototypes, you can think of?

- Materials in Manufacturing (or generically Science in Manufacturing) training camps
- NSF-sponsored projects related to use-inspired research and manufacturing for FIRST Robotics, Girl Scouts of America, Boy Scouts of America, regional science fairs, etc.
- Manufacturer-sponsored senior capstone projects
- National public service announcements on manufacturing’s role in enabling “cool technologies”

- STEMM initiative: Science, Technology, Engineering, Math, **Manufacturing** in US Public School system
- Establish scholarship fund (high school, college, grad school) for individuals to serve as "Science Influencers" or "Manufacturing Influencers" on social media; Similar non-funded programs to be started with early-career professors/manufacturers
- Establish program for early-career sabbaticals for tenure track faculty to spend 9 months - 1 year working at a manufacturing organization
- Altered funding paradigm by NSF and others to heavily prioritize public-private partnerships
- Coordinate with ABET or other accreditors to require inclusion of college course on technology communication in STEMM degrees

What are major milestones? How will we know we are "on track"?

- Increase in number of individuals entering college for science, technology, engineering, math, and manufacturing degrees, particularly women and people of color
- Reduced attrition in STEM**M** degrees/professions
- Increased and positive media exposure on STEM**M** topics
- Reduction in time to commercialize new technology by 30%
- Reduction in global footprint of manufacturing process (appropriate metric? 40%? Increase in onshoring activities by 25%?)

For the remaining questions, imagine that you are all part of a Convergence Accelerator team funded by NSF to address one of the barriers or lead to one of the impacts above. You have three years of significant funding to make a difference.

What does your team composition look like? What kind of skills, backgrounds, expertise are involved?

Data security/infrastructure experts, experts in inter-organizational collaboration, domain experts from industry and academia

Representatives from major R&D participants with different data sharing policies and restrictions:

- industrial participants willing to share problems,
- public and private academic groups/universities
- Government labs, DOD, NNSA, BES

What are three measurable results your team is working towards? It may help to use the SMART framework -- goals should be Specific, Measurable, Attainable, Relevant and Time-Based.

6 month goal:
-Lower the barriers to industry-sponsored capstone projects (what are critical questions interesting to industry, scope, what can be accomplished in a semester?)
-MOU between industry and university consortium
-Establish a two-way "residence program" between the University and Industry

-Initial cadre of projects launched

1.5 year goal:
-XX ongoing projects sponsored by manufacturers
-Identify data format needed by manufacturers for end use applications
-Researchers translate basic R&D results into formats useable and accessible to industry

3 year goal:
-Common database for sharing & receiving and openly disseminating access to industry-sponsored R&D data, models, and codes (e.g. craedl.org)
-Leverage common data base to advertise material capabilities to purchasers, educators, and media partners to help drive material innovation.

How does the technical and organizational diversity of the team improve your ability to achieve these goals? In other words, why is this a Convergence project?
-Building a robust system for sharing data requires accommodating the specific practical and policy restrictions of all R&D stakeholders (national and international industries, governments, public and private universities)

How would this team's work connect to or leverage other initiatives or programs? Examples include other NSF programs, other funding agencies or governmental organizations, or non-profit or international efforts.

Expand framework established by U.S. Manufacturing Innovation Institutes, i.e., LIFT, or Auto/Steel partnership to more broadly address manufacturing and sharing of data

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