NISTIR 8038

Materials Genome Initiative: Materials Data

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January, 2015

U.S. Department of Commerce
Penny Pritzker, Secretary

National Institute of Standards and Technology
Willie May, Acting Under Secretary of Commerce for Standards and Technology and Acting Director

Workshop Summary:

Materials Genome Initiative: Materials Data

15 - 16 July 2014

Dayton, Ohio

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Introduction

key objective for the Materials Genome Initiative (MGI) is access to digital materials data. Access may be for an individual, a team, company, or an entire community of interest. There are several challenges to providing access to digital materials data for which there are presently no universally accepted best practices. Under the MGI, Federal agencies have funded research and development designed to explore, develop, and apply MGI methodologies. Several of these efforts either focus on an infrastructure for sharing data, or emphasize data sharing as a key requirement of the overall technical effort.

One objective of starting several MGI-focused programs concurrently was that the approaches, lessons learned, and best practices would be shared between programs in order to accelerate the overall development of a materials innovation infrastructure (MII). This workshop assembled representatives from Federally funded efforts where a critical component of the overall research effort involves sharing of materials data in digital format. The intent of this workshop was for the participants to provide insights into the goals of their effort, details of their approach to sharing digital materials data, challenges they face, and lessons learned. This exchange of ideas will not only enhance the likelihood for success of the individual efforts, but will also speed the community's understanding of how best to proceed in developing an MII.

During the workshop, participants were asked to identify the top three next steps needed to be taken within the materials community and by government agencies in addressing the challenges associated with digital materials data. The following is list of priorities, derived from those inputs, for each sector

Community

- Develop and deploy standards for data and federated/collaborative environments
- Communicate value and need for digital materials data
- Define critical data to be compiled
- Engage Community
- Explore and leverage data solutions developed outside materials community
- Train students in these emerging areas
- Establish community norms for publishing materials data

Government

- Lead data strategy/approach development
- Incentivize data deposition
- Facilitate data deposition (policy and technology)
- Support data sharing and deposition (provide resources)
- Support data creation
- Enhance data management competency
- Provide quality datasets for model development/validation

MGI Materials Data Workshop Organizing Committee

<u>Air Force Research Laboratory (AFRL)</u>

Dr. Charles Ward & Mr. Clare Paul

<u>Army Research Laboratory (ARL)</u>

Dr. John Beatty & Mr. Wayne Ziegler

<u>Energy Efficiency and Renewable Energy, Department of Energy (DOE-EERE)</u>

Mr. William Joost

<u>National Aeronautics and Space Administration (NASA)</u>

Dr. Stephen Smith & Dr. Dennis Griffin

<u>National Institute of Standards and Technology (NIST)</u>

Dr. James Warren

<u>Office of Naval Research (ONR)</u>

Dr. William Mullins & Dr. Kenny Lipkowitz

Agenda

MGI Materials Data Workshop

Tec^Edge, 5000 Springfield Street, Dayton, OH

1 - 16 July 2014

Tuesday

074 – 0800 Check-in

080 – 0815 Chuck Ward (AFRL) – Introductory remarks

Discussion Lead: Will Joost (DOE-EERE)

081 – 0845 Jim Warren (NIST) – Data Infrastructure

084 – 0915 John Allison / Brian Puchala (Univ. Michigan) – PRISMS/ALMMII

091 – 0945 Carrie Campbell (NIST) – ChiMaD

094 – 1015 *Discussion*

101 – 1030 *Break*

Discussion Lead: John Beatty (ARL)

103 – 1100 Marco Fornari (Central Michigan Univ.) - AFLOWLIB.org

110 – 1130 Surya Kalidindi (Ga Tech) – Mosaic of Microstructure/IGERT-CIF21

113 – 1200 *Discussion*

120 – 1230 *Lunch*

Discussion Lead: Bill Mullins (ONR)

123 – 1300 Tom Searles (MDMi) – Cast Aluminum

130 – 1320 Dongwon Shin (Oak Ridge National Laboratory, ORNL) – Cast Aluminum

132 – 1340 Jake Zindel (Ford Motor Co.) – Cast Aluminum

134 – 1415 *Discussion*

141 – 1430 *Break*

Discussion Lead: Jim Warren (NIST)

143 - 1500 Jason Sebastian (Questek) – Cast Iron

150 – 1530 Lou Hector (General Motors) – Advanced Steel

153 – 1600 Lara Liou (GE Aviation) - Integrated Computational Methods for Composite Materials

160 – 1700 *Discussion*

1700 Adjourn for the day

Wednesday

074 – 0800 Check-in

Discussion Lead: Wayne Zeigler (ARL)

080 – 0830 Terry Wong (Rocketdyne) – Nickel RS FEP

083 – 0850 Mike Glavicic (Rolls Royce) – MAI Ti Modeling

085 – 0910 Rajiv Naik (Pratt & Whitney) – MAI Data Informatics, Data Standards, Modeling & UQ

091 – 0940 *Discussion*

094 – 0955 *Break*

Discussion Lead: Dennis Griffin (NASA)

095 – 1015 Ro Gorham (National Center for Defense Manufacturing and Machining, NCDMM) – America Makes

101 – 1045 Richard Serwecki (NASA) - MAPTIS

104 – 1105 Scott Henry (ASM International) - Computational Materials Data Network

110 – 1135 *Discussion*

113 – 1200 *Lunch*

Discussion Lead: Clare Paul (AFRL)

120 – 1230 Ben Blaiszik (Univ of Chicago/ANL) - Globus

123 – 1300 Mike Groeber (AFRL) – DREAM.3D/SIMPL

130 – 1320 Sam Chance (iNovex) - Semantics for Deep Interoperability

132 – 1340 Harlan Shober (RJ Lee) - Big Data and Semantic Technologies

134 – 1400 Tim Hawes (Decisive Analytics Corp) – Natural Language Processing

140 – 1445 *Discussion*

144 – 1500 Wrap up

1500 Adjourn

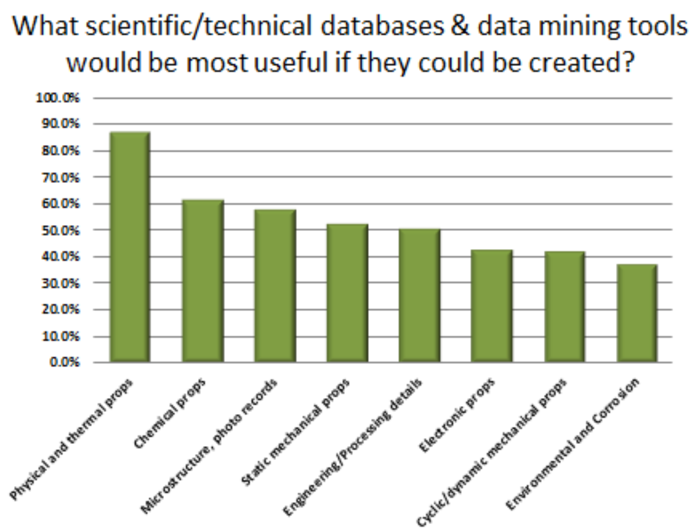
Presentation Summaries

Welcome and Introduction

Chuck Ward, Air Force Research Laboratory

The primary intent of the workshop is to promote communication between the groups being funded under the Materials Genome Initiative that had significant interest in the management of materials data. The greater awareness is expected to enhance the likelihood for success of the individual efforts and speed the community's understanding of how best to proceed in developing an MII.

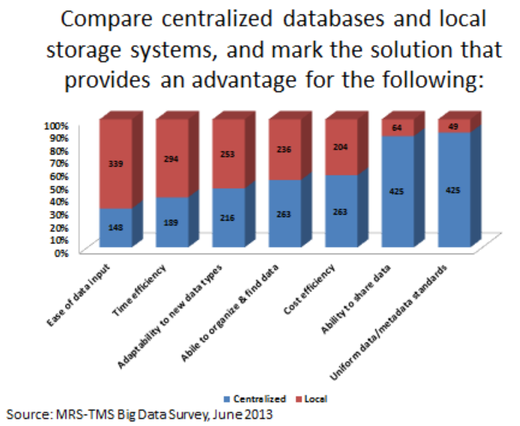
The Materials Research Society (MRS) and the Minerals, Metals, and Materials Society (TMS) conducted a survey of the community in May/June of 2013 to gauge attitudes and needs in materials data. Over 650 people took the survey, with 74% of respondents saying they would be willing to share data if it were encouraged as a condition of funding or publishing. The community showed the most interest in gaining access to databases of some of the most basic and essential materials data, such as thermo-physical properties.

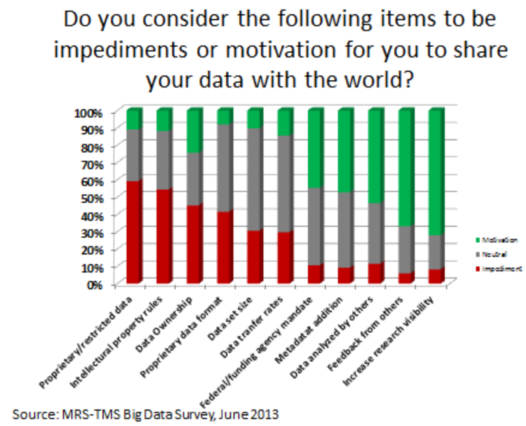


Source: MRS-TMS Big Data Survey, June 2013

The survey asked participants to evaluate advantages of local versus centralized databases. Centralized repositories were perceived by respondents to offer advantages in cost, an ability to share one's data, provisioning of uniform data standards, and an ability to organize and find data. Local repositories were perceived to provide advantages in ease of data input, time efficiency and flexibility in accommodating new data types.

The survey also asked participants to provide their thoughts on impediments to and motivators for sharing data. Most of the impediments can be attributed to concerns of ownership of data or external data restrictions while technical issues such as file size and proprietary formatting were also concerns. Overall, participants saw the ability to contribute data to the community for reuse and critique positively. The highest motivator was to enhance one's own research visibility. Interestingly respondents saw adding metadata as a motivator, presumably due to the perceived higher value of data when it is described more robustly.





MGI Efforts in Infrastructure Development at NIST

Jim Warren, National Institute of Standards and Technology

The presentation provided an overview of NIST activities supporting the creation of a materials data infrastructure. The infrastructure could start by defining the interfaces/APIs (Application Programing Interfaces) with which user is able to interact for the deposit or retrieval of data. Beyond an interface, the following are essential elements for creation of viable infrastructure:

- The establishment of repositories to store the data
- Tools to enable digital capture of the information, preferably at the time of creation (computation or experiment)
- Tools to enable markup of the data with sufficient metadata to inform someone else how the data was created, as well as various attributes that would help the user judge the quality of the information
- Assignment of a persistent digital identifier (like the DOI (Digital Object Identifier) for journals) so the data can be cited and discovered by other
- The registration of the availability of the data into some sort of "registry" to enable discovery without prior knowledge of the existence of the repository/specific data features

Additionally, creation of new policy and standards as well as development of tools to evaluate the quality of the data and tools to enable data-driven discovery will be required to manage and use materials data to the greatest extent possible.

NIST is responding to the OSTP (Office of Science and Technology and Policy) memos (Dr. John Holdren, 2 Feb 14) by developing practices that will be of use to the community including a Common Access Platform allowing access across multiple collections of information, Research and Development of Persistent Identifier (PID) infrastructure with the Research Data Alliance (RDA), and R&D o Data Type Registries with RDA.

Finally, NIST is collaborating with the National Data Service (based at the National Center for Supercomputing Applications) and is developing a set of best practices for Data Management Plans.

Th Materials Commons: A Novel Information Repository and Collaboration Platform for the Materials Community

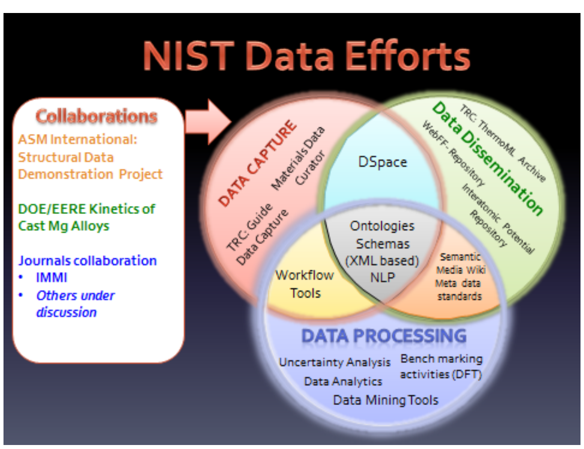
Brian Puchala, Glenn Tarcea, Stravya Tamma, Emmanuelle Marquis, John Allison, University of Michigan

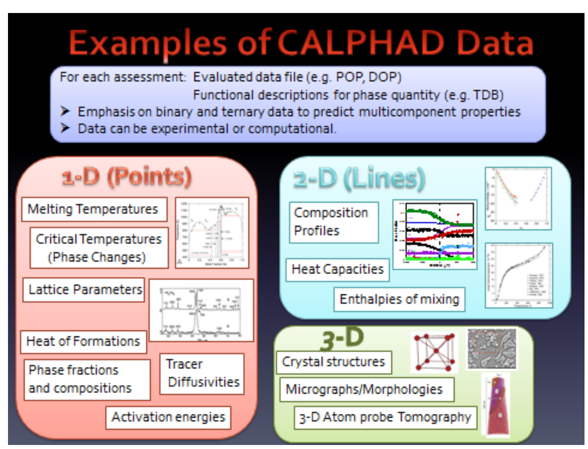
Critical to accelerating the pace of materials science and development is the development of new and improved infrastructure providing a seamless way for materials researchers to share and use materials data and models. To address this need, we are developing the Materials Commons (http://prisms.engin.umich.edu/#/prisms/materialscommons), an information repository and collaboration platform for the metals community in selected technical emphasis areas. We envision the Materials Commons becoming a continuous, seamless part of the scientific workflow process. Researchers will upload the results of experiments and computations as they are performed, automatically where possible, along with the provenance information describing the experimental and computational processes. By associating this data with the experimental and virtual computational materials samples from which it is obtained, the Materials Commons will build process-structure-property relationships enabling the construction and validation of constitutive and process models. The Materials Commons website provides an easy-to-use interface for uploading and downloading data and data provenance, searching, and sharing data. At its core, the Materials Commons consists of secure data storage cluster, an application for efficiently uploading and downloading large data sets, and a REST (REpresentational State Transfer) based API to access and extend the capabilities of the repository. The API allows for features such as automated data upload from experiments and computations, seamless integration of computational models, and algorithmic analysis of process-structure-property relationships. The Materials Commons is a central thrust of the Center for PRedictive Structural Materials Science (PRISMS).

NIST Materials Data Informatics Efforts

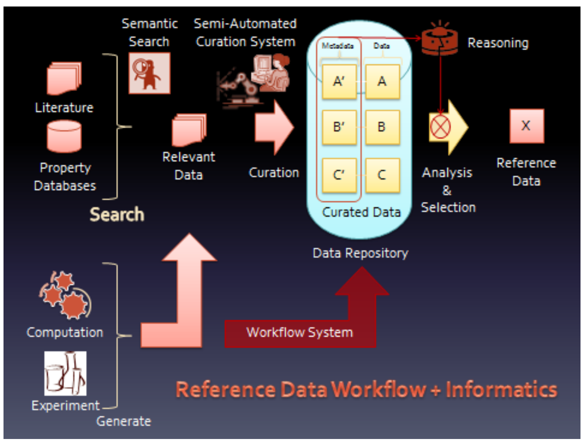
Carrie Campbell, National Institute of Standards an Technology

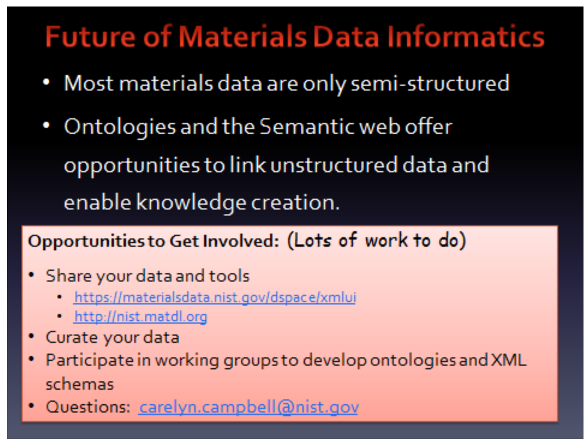
The presentation covered NIST's pilot efforts in creating a data infrastructure, focusing on Phase-Based Property Data. Phase-based data are diverse data that include 1, 2, 3, and 4-dimensional data, are semi-structured and often include incomplete data sets.   The figure below provides an overview of NISTs data efforts supporting the MGI.





NIST Materials Data Repository (https://materialsdata.nist.gov/dspace/xmlui) is a customized DSpace repository for materials that enables sharing of variety of data types, including text files, images, and video. The repository also provides persistent identifier for each entry and allows users to choose from a variety of license types. NIST is also working on two data curation tools for phase-based data. The Thermodynamic Research Center (http://trc.nist.gov/) is extending the ThermoML markup language and Guide Data Capture software tool to metallic systems, with an initial emphasis on phase equilibria and thermochemical data. The Materials Data Curation System (MDCS) employs user-defined XML-based schemas to curate data. The MDCS allows either web-base data curation or using REST API. The entered data is stored in a non-relational database repository, can be searched using SPARQL (SPARQL Protocol and RDF Query Language*)* interface, and integrated with variety of scientific workflow tools.





AFLOW Consortium

Marco Fornari, Michigan State University

The overall goal of the Materials Genome Initiative (MGI) is to accelerate the discovery, development, and deployment of new materials with ad hoc functionalities. The AFLOW Consortium focuses on the software infrastructures to achieve the MGI goals by using first principles calculations. The emphasis is on the data that must be generated, archived, validated, and post-processed efficiently both to identify new materials and distill meaningful quantitative relationships within the data. This extends the solution to the inverse problem of chemically replacing rare and costly elements in critical technologies.

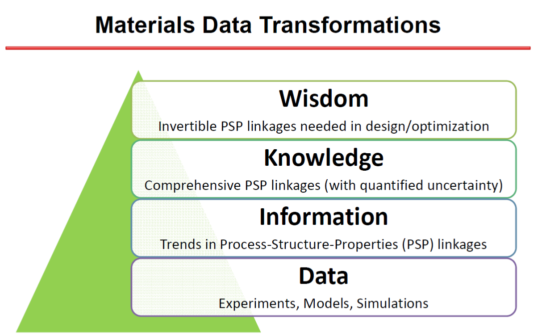
The AFLOW Consortium provides access to the repository AFLOWLIB.ORG <http://AFLOWLIB.ORG> that publicly distributes data on energetics and thermodynamic stability for more than 600,000 compounds and band structures for roughly 300,000 materials. The repository includes bulk crystals and alloys. Data were computed with the AFLOW high-throughput framework using density functional theory. The results of the calculations can be queried with the recently developed REST-API that standardizes and labels the data for retrieval purposes. The fields defined in the AFLOW REST-API include a material object identifier (AUID), data cloud location (AURL), ownership and sponsorship keywords, and data specific labels (COMPOSITION, ENTROPY, EGAP, …). Simple scripting languages can be used to automatically download from the AFLOWLIB repository. The AFLOW approach has been extensively applied on Platinum-group alloys, thermoelectric materials, magnetic materials, topological insulators, scintillators, etc. The AFLOW REST-API can be extended to include experimental data. For further details on the database, the reader is directed to: http://materials.duke.edu/auro/AUROARTICULA/j.commatsci.2012.02.002.pdf

Materials Innovation Infrastructure: Lessons Learned and Future Plans

Surya Kalidindi, Georgia Institute of Technology

central activity in materials research is the exploration of processing-structure-property (PSP) linkages. W*orkflow* is defined as the sequence of steps employed for establishing PS linkages of interest to any specific engineering/technology application.

High Throughput Explorations of PSP Linkages: We must treat hierarchical material as a complex System, which means embracing and exploiting uncertainty quantification and complexity management concepts/tools. It also means we need to design, develop, and validate decision support systems that will leverage the best current understanding (with its uncertainties) and provide objective guidance on future effort investment (combination of experiments and simulations). This means leveraging Data Science to effectively feed the decision support systems described above by developing and deploying high throughput strategies for obtaining high value information from both experiments and models.



Integrated workflows are needed to objectively extract knowledge and wisdom from raw data

What are integrated workflows? Integrated workflows are those that utilize the best combination of experiments and simulations in extracting robust and reliable PSP linkages. This requires engaging and exploiting cross-disciplinary expertise that includes materials science, manufacturing, systems approaches, uncertainty quantification, computational science, data and information sciences. Through this, one must ensure that the workflows output the critical information needed by design and manufacturing stakeholders in the materials development value chain. *Integration demands expertise sharing, which essentially is the core element of a collaboration. Cross-disciplinary Integration demands effective collaborations, such as those one might set up using the modern tools of the day, i.e., a e-Collaboration.*

Motivators for e-Collaborations: e-Collaborations are central to enhancing the productivity of materials development activities in several ways:

- individual research groups can identify and engage complementary expertise needed for their projects
- organizations can coordinate multiple teams and multiple projects to maximize output/impact
- organizations can identify and seek the right partners that enhance their individual and combined value.

e-Collaborations can be open, semi-open, or closed depending o the needs of the specific organization. Productivity enhancement leading to dramatic reductions in cost and time expended in materials development is the main incentive for e-collaborations.

Main Impediments to e-Collaborations:

Lack of tools to identify the "best" collaborators

- Need software tools that quantify more precisely the expertise of individuals, groups, organizations
- Need software tools for allowing rich annotations and e-recording of discussions. Need analytic tools for identification, extraction, and management of metadata (i.e., high value abstractions from the raw data)
- Need searchable, semantic, metadata databases (these are lightweight and can be centralized and customized for specific user communities)
- Need software tools for tracking provenance (i.e., who/what/when/how generated, modified, etc.)

Lack of experience with the use of integrated workflows

- Need software tools for e-recording of workflows and development of searchable workflow databases
- Need recommendation schemes that suggest the best workflow(s) based on recorded prior experience; this provides means to transfer expertise acquired by an organization to other teams and other projects (even in the same organization)
- Leads to possible automation and dramatic enhancement of productivity

MINED Group's Past Experience: (~2005 - ~2008): Funded by the Army Research Office, ARO, (David Stepp); engaged computer science (CS) graduates to produce a single user platform that integrated certain software codes previously produced by our group; software development subsequently abandoned, but recruited two CS graduates into PhD programs in Materials Science and Engineering/Mechanical Engineering (MSE/ME), which dramatically altered the direction of research in the group. brief chronology of development:

- Senior Design Project (2011-2012): An online portal designed for sharing data files and tools; learned the importance of user interfaces and the need for professional code developers and software architects.
- HUBzero Instantiation (2012-2013): Built hub by customizing HUBzero for hierarchical structural materials; there are several advantages in terms of accessing and executing codes (on the server side), but there are significant barriers to establishing fast and productive cross-disciplinary e-collaborations.

- GTRI Integration Platform (2013-2014): Engaged professional code developers and software architects to design a multi-user web portal that allows data and code sharing, while tracking provenance and workflows; underestimated the resources needed for such a project.
- MATIN Collaboration Environment (2013-2014): Lightweight integrated software shell that allows users to seamlessly interface with numerous cloud services offered through the web through their APIs. Examples include GitHub for versioning and archival of codes, Authorea for collaborative editing of documents, figshare for citable publication of research, Plot.ly for collaborative data analysis and visualization, Google+ and LinkedIn for eteaming and networking. MATIN focuses on building an emergent community – Materials & Manufacturing Informatics (MMI). MATIN provisions web services for software, integration platforms, and innovation infrastructure.

  Examples of MATIN:
- Spatial Statistics: https://github.com/tonyfast/SpatialStatisticsFFT
- PyMKS: http://openmaterials.github.io/pymks/index.html
- Example discussion about periodic boundary conditions in running Finite Element (FE or FEM) simulations: https://github.com/sfepy/sfepy/issues/267

In the platform developed, it is noted that the user or user's organization can set permissions at the level of individual datasets/codes o the degree and type of sharing.

Central Challenge: Activation. The transition from traditional disciplinary workflows to the integrated workflows needs to overcome an activation barrier. There is no clear incentive to get ahead of the curve in anticipating how the upcoming transformations in how materials development will be pursued in the future. Open (reproducible) science alone is not a sufficiently strong motivator for materials development community with strong interests in intellectual property development; indeed, it might actually be perceived as a negative. There is need to explore and refine what incentives work for individual researchers (e.g., increased productivity).

Future Plans: Continue to develop and deploy MATIN at GT and any other organizations/groups that express an interest in working with us. Design, create, and distribute suite of "mobile first" Apps designed to make data ingest into collaboration environments such as MATIN from both material characterization equipment and multi-scale models an enhanced user experience with friendly and natural interfaces. Proactively promote/incentivize data/metadata ingest into publicly shared databases. Work with professional societies to announce and run new competitions/awards for recognizing and rewarding good practices by the members of the broader materials innovation user community (e.g., Best Documented Data Award, Best Documented Tool Award, Best Documented Workflow Award). Develop and deliver new workshops for training the new generation of graduate students, postdocs, and junior faculty in the emerging workflows of Materials & Manufacturing Informatics.

High Performance Cast Aluminum Alloys for Next Generation Passenger Vehicle Engines

Dongwon Shin, Materials Science and Technology Division, Oak Ridge National Laboratory

Oak Ridge National Laboratory (ORNL) teamed with Chrysler and Nemak to develop next-generation high-performance cast aluminum alloys that have improved castability, high-temperature strength, and fatigue performance. At this point, the data management practice is limited to analytical data spreadsheets, other than the CALPHAD computational thermodynamic databases and proprietary property databases for casting simulation. As the project goes on, more robust data schema will be developed to store various types of data populated from the experiments and calculations.

Besides the data structure design, the speaker discussed the necessity of a new approach to identifying key descriptors from the large dataset that can guide the design of new materials. An alloy design requires the balance of extremely complex relationships among a large number of descriptors. Some examples of these descriptors include phase fraction of key intermetallics, lattice parameters of the matrix, and diffusion kinetics of solute atoms. However, optimizing these quantities relies on good physical metallurgy intuition coupled with clever experiments, dogged sleuthing, and a healthy dose of luck. Such descriptor-based predictions of materials properties date back to the beginning of modern solid-state chemistry and physics. As shown in the Darken-Gurry map to predict the solubility of elements in Tantalum, intuitive descriptors, such as electronegativity and radius, could be used for materials design. However, as the chemistry and physics of materials become more complex, intuition-based search may not work anymore. Thus, the use of more advanced statistical analysis and data mining approach might be required to accelerate the design of complex multi-component/multi-phase alloy design.

Data Related to Cast Aluminum

Jake Zindel, Ford Motor Company

The main focus of our research is the development of CAE (Computer-aided Engineering) tools to support two significant activities in the company: component design (product development) and manufacturing engineering (high-volume production). A key part of our research is conducting experiments to collect data for the development and validation of the CAE tools.

The data we collect consists of mechanical properties, physical properties, microstructural images, and manufacturing process parameters that form the pedigree of the material. This information can be in the form of Excel files, proprietary-software storage files, screen shots, and written reports.

Our immediate need is to deal with this large amount of existing information, collected over many years, on a “local” level. The first step is to organize many independent collections of information in all their forms. The next issue is the time required to enter all this information into the database. Maintenance may also require a significant amount of effort. Lastly, there will also be a need to manipulate the data contained in the database using Excel, Mini-tab, MATLAB, etc. Therefore links or easy exportation of data to these types of applications will be necessary.

The next level would involve dealing with information that has been created or collected by others. From an OEM (Original Equipment Manufacturer) perspective, this would involve convincing suppliers to share processing information that they may consider proprietary. In addition to suppliers, universities and national laboratories are also sources of data. Data from all the sources will require some sort of protocol to determine its quality and resolve inconsistencies.

In the end, it seems likely that considerable budget and time will be required to implement comprehensive information/databases, which could be the largest hurdle of them all.

QuesTek's MGI/ICME Approach to Alloy Optimization and Design (Including Cast Iron)

Jason Sebastian, QuesTek Innovations LLC

Integrated Computational Materials Engineering (ICME) methods involve the holistic application of different computational models across various length scales to the design, development, and rapid qualification of advanced materials. Using its *Materials by Design* technologies, QuesTek has successfully applied these ICME methods to the design, development, and full qualification of several advanced alloys (including aerospace structural steels, aerospace gear steels, advanced castable titanium alloys, high-strength, corrosion-resistant aluminum alloys, and high-performance cast iron).

QuesTek's ICME methods benefit tremendously from the activities of the U.S. Materials Genome Initiative (MGI). Recognizing that the "10 to 2 years" that it takes for alloy design and development is hindering the rapid deployment of higher-performance materials, the MGI is focused on "cutting in half" the time and cost to design and deploy novel, advanced materials needed to enhance and sustain U.S. competitiveness.

QuesTek also has ongoing activities on the application of ICME methods to the design and development of materials for the energy sector, including advanced materials that enable vehicle lightweighting. Of particular note is an ongoing effort with a major diesel engine manufacturer on the development of high-performance cast iron alloys for engine block applications. QuesTek's efforts have made extensive use of various MGI-type tools and databases including: 1) density functional theory methods for high-throughput screening of cast iron inoculant stabilities (structure, lattice parameter, stability of various oxide/sulfide phases), 2) liquid iron mobility databases (to help accurately model solidification phenomena), and 3) thermodynamic databases (to examine nano-precipitate stability).

Moving forward, to continue to accelerate the materials development cycle, efforts should remain focused on the development of the fundamental databases (thermodynamic, kinetic, etc.) that enable ICME models. There should also be increased focus o efforts related to the integration of the various computational databases, models, and tools (the "I" in ICME).

Integrated Computational Materials Engineering (ICME) of Generation Three Advanced High Strength Steels

Louis G. Hector, Jr., General Motors R&D Center

While traditional material development methods often involve laborious trial-and-error testing, Integrated Computational Materials Engineering (ICME), which falls under the umbrella of the Materials Genome Initiative, is offering a means for materials development under a more compressed time scale. Advanced high strength steels (AHSS), which contain multiple phases (e.g., ferrite, bainite, pearlite, austenite, martensite), and may exhibit phase transformation with strain, are fertile ground for ICME. However, prediction of macro-scale constitutive behavior based upon the multi-scale physical, chemical, and mechanical phenomena in these complex microstructures is formidable challenge for ICME. Unprecedented collaboration between universities, industry, and government labs will be required to address AHSS development, archiving of data, and the implementation of these materials into products that benefit the American consumer. This presentation began with a brief overview of a new, DOE/USAMP (US Automotive Materials Partnership)-funded ICME program aimed at the development of Generation Three (Gen 3) AHSS. The lack of commercial Gen 3 steels that meet DOE targets is offering significant challenges to this new ICME program. The program is meeting these challenges following four thrusts: (1) making Gen 3 steels to meet DOE targets; (2) passing experimental measurements of key properties to an ICME model that produces microstructure-based constitutive models; (3) material evaluation in forming and vehicle performance simulations; (4) archiving all relevant data for easy use by others in the program. Although the Gen 3 AHSS ICME program is "mission oriented," it demonstrates an important role for universities in providing the necessary foundation in fundamental materials science and engineering.

Integrated Computational Methods for Composites Materials (ICM2): Lessons Learned from Integration Planning and Feasibility Demonstrations
Lara Liou, GE Aviation

General Electric Aviation and Lockheed Martin Aeronautics have teamed through an Air Force Research Lab program to conduct a demonstration of an Integrated Computational Materials Engineering digital framework that links material processing, property, and structural relationships to account for processability, manufacturability, and system performance with the goal of demonstrating that the usage of integrated models can contribute to future airframe and engine designs with dramatic reductions in development time and cost. Both engine and airframe Foundational Engineering Problems will be demonstrated through a common digital framework to be developed and validated on increasingly complex articles. The modeling tools that cover composite process models, localized mechanical behavior models, and global design models (Convergent Manufacturing Technology's COMPRO CCA, Autodesk's Autodesk Simulation Composite Analysis, and an Abaqus based University of Michigan micromechanics model) are centrally linked via a commercially available model integration interface (Phoenix Integration's ModelCenter®). Detailed plans of what data will be passed among the various models as well as how it will be passed have been completed. Creation of these detailed process maps and simple feasibility demonstrations have raised inherent technical and logistical challenges to integrating commercially available, multi-scale models. Robust model integration methods to address these challenges were discussed.

The exercise of drawing up detailed process maps for what to integrate and how to integrate the selected tools and models resulted in key early lessons learned and identification of tools critical to long-term, robust, and sustained application of Integrated Computational Methods for Composites Materials (ICM2). The key lessons learned include:

- Individual models must be relatively mature and validated before an ICM2 problem can be confidently defined.
- F analysis-based tools within the same digital thread should utilize the same FE solver.
- The team, ideally, should consist of at least one expert for each tool and its underlying model as well as an expert in the digital thread and integration interface tools and programming.

- Mesh interpolation between finite element analysis based tools will likely be required, and a commercially available tool for this type of composite mesh interpolation is key for robust and sustained application of ICM2.

Residual Stress Engineering of Rotating Nickel Components

Terry Wong, Aerojet Rocketdyne

The goal for the PW-8 project: The Nickel Base Superalloy Residual Stress Foundational Engineering Problem program aims to develop a multi-disciplinary analysis approach to predict and incorporate bulk residual stress in the design of component. This will allow for design of part that is optimized for a particular application or design intent (such as weight, performance, or reduction of scrap). To accomplish this goal, the PW-8 team has two major tasks; 1) the development of an infrastructure and associated tools needed to predict and incorporate bulk residual stress in the design stages of a part, and 2) a demonstration task that will validate the infrastructures and tools developed.

The Data Management task is the foundational element of the larger infrastructure development task. The goal for the data management work is to develop an infrastructure that allows the various team members in PW-8 to share data and to store data in database. This not only ensures that data generated by this program is never lost but also allows for data to be transferred in a secure manner. In order to meet the goal of a system that securely stores and shares data, three major tasks must be accomplished: 1) Validation that there is secure method to transfer data between team members and that the method of storing data is also secure, 2) development of a database schema and 3) development of means to easily upload data into the database and download data from the database.

Of the three, the most difficult task was to create a system in which the transfer and storage of data was secure. Various proposals were made to ensure the security of the data but many of them were rejected, not because the proposal was actually unsecure, but because it was not acceptable by each of the team member's IT security policies. The process to get each team members' IT department to approve the security of the data transfer and storage took more effort than anticipated. In the end, the team members along with their respective IT departments approved the use of TRUcentrix as a tool to transfer data and the use of an ASM International hosted database to store data.

The development of database schema is necessary step in creating the database to store all the data generated (via physical tests as well as data generated by models). A big help in creating the database schema was to use the schema generated by Dr. Steven Arnold from NASA's Glenn Research Center. Using NASA's schema eliminated the need to start the database build from scratch and allowed us to focus o the specific needs of storing residual stress data.

The last task involves the development of tools that make the input of data easy. The more difficult it is to enter data into a database, the more likely data will not be entered. Excel-based templates are being developed in order to make data entry as easy as possible.

The two big lessons learned from PW-8 in relationship to data management are:

- It is essential to work with each companies' IT and IT Security people to develop a system that satisfies the security requirements of each company.

- Database schema development should not be reinvented but begin with already established the schema.

Perspectives on MAI Programs

Dr. Mike Glavicic, Rolls Royce

The current formulation of MAI (AFRL's Metals Affordability Initiative) programs are structured independently from one another in that a standard methodology does not exist that describes what data is to be archived at the conclusion of a program. Nor does there exist a standard protocol of how to archive things on a server or some other computer resource at the conclusion of a program. As a result, the current practices of MAI programs:

- Do not address IP (intellectual property) and licensing issues in systematic fashion, which leads to issues in the commercialization of ICME software that is generated under a program

- Do not have a formalized requirement of how data is to be packaged and stored at the end of a program. Hence even in the best of cases in which all of the data is stored, the data is archived in simple folder fashion that is not searchable in any manner possible. Moreover, even if all of the data is present it is extremely cumbersome to untangle the data for future use using a file folder strategy.

Hence at the end of the program both the government and MAI team are left to manage the data and results in an unregimented fashion.

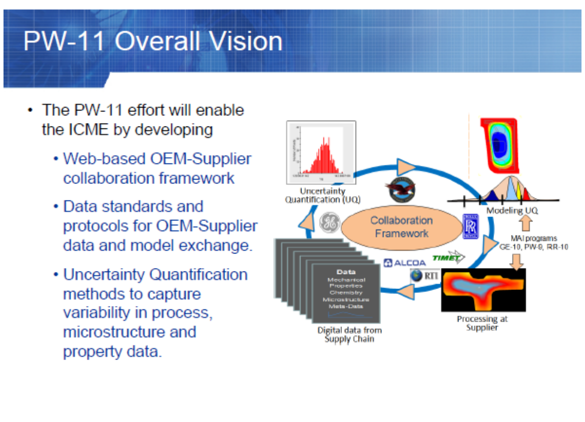
The lack of regimented protocol of how to package program's results (raw data and reports) makes it extremely difficult for new government programs to leverage the data from previous programs. Case in point, the RR-10 program was developed with the singular goal to integrate the models developed in the LAD-2 program into commercial software platform. From the outset of the program, data, models and other information that was required to attained the goals of the RR-10 program were either difficult to track down, lost or not provided to the RR-10 team due to contractual disputes. As a result, funding that was earmarked for specific technical work at the conception of the program had to be diverted for the recreation of data that existed in a previous program and the progress of the program was stunted by this unforeseen burden. In spite of the RR-10 program's ability to overcome these issues and become a successful program, it should be noted that the success of other programs that will encounter similar problems will likely not apply as RR-10 was very fortunate to have the means to overcome these serious issues that were a result of the lack of a data management plan.

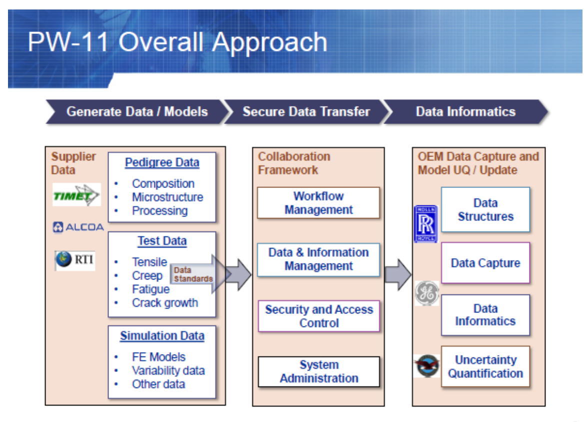
Furthermore, if the MGI initiative is to progressively develop materials models that are leveraged and improved in future government funded programs a policy on how to store and share the data from disconnected programs is required. The PW-11 program is the first step in this process as it will have the data from three MAI programs (RR-10, GE-10, PW-9) uploaded into database that will be searchable and will enable the reuse of the data collected in these programs. However, even if this program is a success there will undoubtedly be other features that will be required in the platform developed and hence future modification will be required. Most importantly there does not currently exist server that has been set up and funded for the archiving of all future programs with a protocol that must be adhered to at the conclusion of a funded program. Without such a protocol and the existence of server to be used in all future programs, the goals set forth by MGI will be unnecessarily difficult and more expensive to attain.

MAI Data Informatics, Data Standards, Modeling & UQ

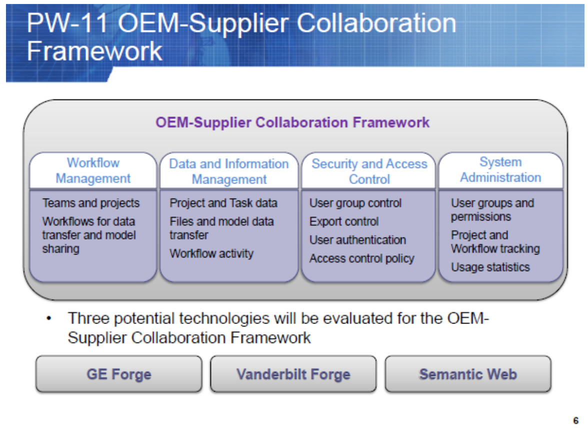
Dr. Rajiv Naik, Pratt & Whitney

The MAI Data Informatics, Data Standards, Modeling & Uncertainty Quantification (UQ) (PW-11) effort will enable the pervasive implementation of ICME by developing (i) a web-based OEM-Supplier collaboration framework for production certification and process modeling data, (ii) data standards and protocols for interoperability between OEMs and Suppliers, and (iii) UQ methods to capture variability in process, microstructure, and property data. Models and data from earlier MAI programs such as GE-10, PW-9 and RR-10 will be used to develop and implement OEM-Supplier integration, data standards, data structures, and UQ models. Several OEMs and suppliers (Pratt & Whitney, General Electric, Rolls-Royce, TIMET, Alcoa and RTI International Metals, Inc.) are working together on the PW-11 Team.





The OEM-Supplier collaboration tool will enable data exchange related to mechanical testing, microstructural characteristics, processing, and process modeling. The data standards developed by the PW-11 team will provide an industry standard for such OEM-Supplier collaboration. The collaboration framework would provide a platform to manage OEM-Supplier workflows, data and information, security and access control, and the ability to perform system administration without the need for day-to-day intervention of the IT department. The capture of such supplier data over the collaboration framework will enable the OEMs to enhance process and property models, data analytics, and UQ modeling. Three potential technologies will be evaluated for the OEM-Supplier Collaboration Framework – GE Forge, Vanderbilt Forge, and Semantic Web technology and one technology will be selected for the next phase of the program.



Semantic Web technology is paradigm shift from highly structured databases to more flexible graph databases, from single database searches to multiple and disparate database searches, and from keyword searches to contextual and meaningful (semantic) searches. It can provide flexibility of data structures and enhanced OEM-Supplier interoperability. However, it requires more work upfront for implementation as it needs the development of a common vocabulary and relationships.

The data standards and data structures effort will leverage work at national and international standards organizations such as ASM, ASTM, CEN, and NIST and develop standards and vocabularies for production certification data that can include chemistry, microstructure, and mechanical properties. This effort will also develop means for the capture of data needed for the UQ and ICME models and build databases for the capture of the data from the GE-10, PW-9, and RR-10 MAI programs.

The ICME models being developed under the GE-10, PW-9, and RR-10 programs involve several interconnected models related to processing, microstructure and mechanical properties. The UQ effort under PW-11 will involve considering the uncertainty at each step of the modeling process and flowing it through the interconnected models to evaluate the relationships between the variabilities of the processing parameters, the microstructure and the mechanical performance.

ASM's Computational Materials Data Network & the NIST-ASM Structural Materials Data Demonstration Project

Scott D. Henry, ASM International

ASM International – the world's largest association of metals-focused materials engineers, scientists, technicians, educators, and students – has launched a series of initiatives under the "Computational Materials Data (CMD) Network" umbrella. The objective of the CMD Network is to serve as center for information collection and dissemination for materials data to support integrated computational materials engineering (ICME) and to help realize the goals of the U.S. Materials Genome Initiative.

The first major project for the CMD Network is the NIST-ASM Structural Materials Data Demonstration Project (SMDDP), a cooperative research project funded by NIST with participation from the Kent State Center for Materials Informatics and Granta Design Ltd. The main objectives of SMDDP are to:

- Establish well-pedigreed and curated demonstration datasets for non-proprietary metallic structural materials data over multiple length scales. The team has chosen to work with 6061 aluminum and the related Al-Mg-Si system.

- Work with NIST and the materials data community to develop materials data schema and ontologies for the demonstration datasets, cognizant of broader interests and datasets.

- Develop and carry out a series of test problems that represent relevant use cases for the repository.

- Make data open to the materials data community for use in data analytics, modeling, and educational purposes.

- Actively engage the materials data community and widely disseminate the findings from the project.

- Develop and implement data capture and curation procedures that can serve as models for other data repositories.

The basic philosophy behind the project is that often standards emerge through trial and error, and examples are needed to spur this process.

The project is using the NIST-KSU DSpace repository for data files. The curated, structured database is being developed using GRANTA MI software and is hosted o ASM servers.

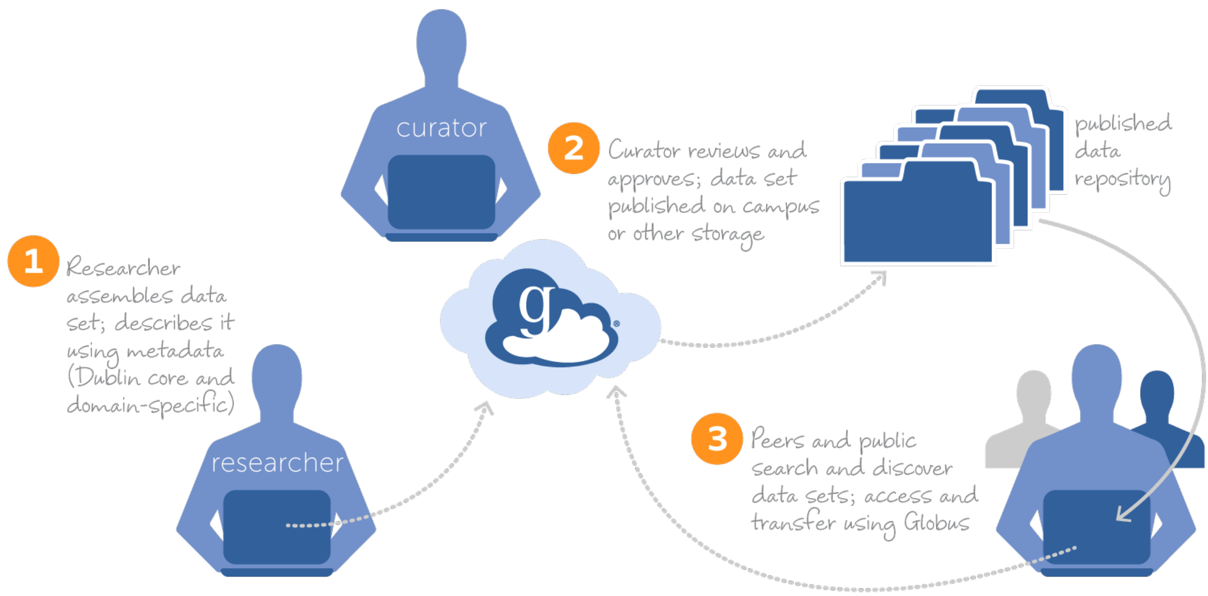
The project –launched in late 2013 and planned as an 18-month program – is being conducted in phases. The first phase involved developing starter database and gaining experience in data curation. The second phase (currently underway) involves building out more comprehensive data sets that will be suitable for carrying out test problems related to processing-structure-property relationships in Al 6061. The third phase will involve making further refinements in response to testing. The complete data set will be opened up online to the materials community as a whole.

Globus Scientific Data Services: Current and Future

Ben Blaiszik[1] Kyle Chard[1] Jim Pruyne[1], Rachana Anathakrishnan[1], Steve Tuecke[1,2], Ian Foster[1,2]
[1]University of Chicago Computation Institute, [2]Argonne National Laboratory MCS Division

During this talk, we discussed a variety of currently available Globus services. Via these Globus services, developers and IT administrators can offer simple, secure, and robust file transfer, as well as identity, profile, and group management to their user communities. Globus allows end users to create and manage a unique identity that can be linked to external identities for authentication. End users can also transfer files across wide area networks faster and more easily, whatever their location.

The talk also covered prototype services related to data publication, metadata tagging, and data search. Globus publishing capabilities are delivered through a hosted service. Metadata is stored in the cloud, while raw published data and a fully-formed metadata log are stored on campus, institutional, and group resources that are managed and operated by campus administrators. Published datasets are organized by "communities" and their member "collections". Globus users can create and manage their own communities and collections through the data publication service with collection level policies regarding user access. Additionally, metadata from these communities are imported into a centralized index to allow for robust searching functionality.



Semantics for Deep Interoperability

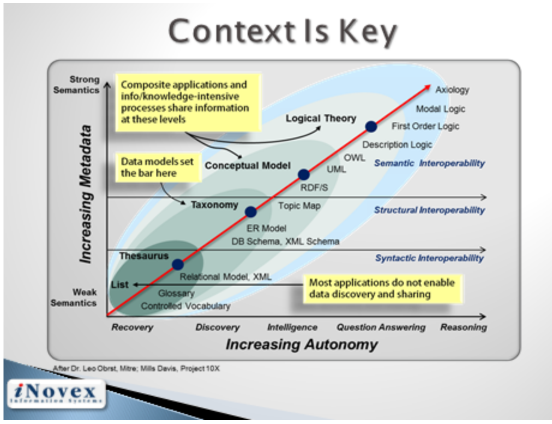
Samuel Chance, iNovex

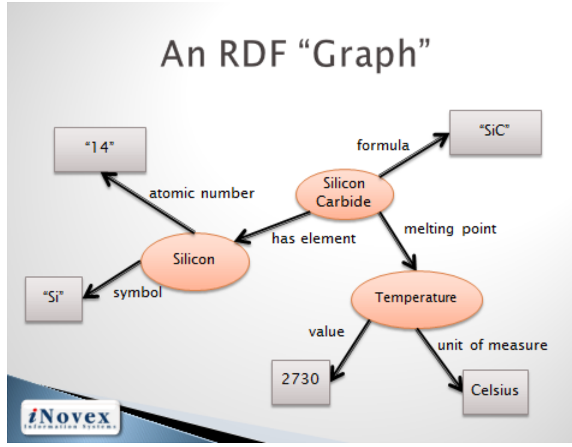
Semantic technology is based on mature web standards and intended to be used as global framework for machine-to-machine communication. Interoperability is enabled even when the more basic elements of the semantic technology stack are used in conjunction with a controlled vocabulary. Knowledge representation is enabled as one begins to utilize the “higher” elements of the stack.

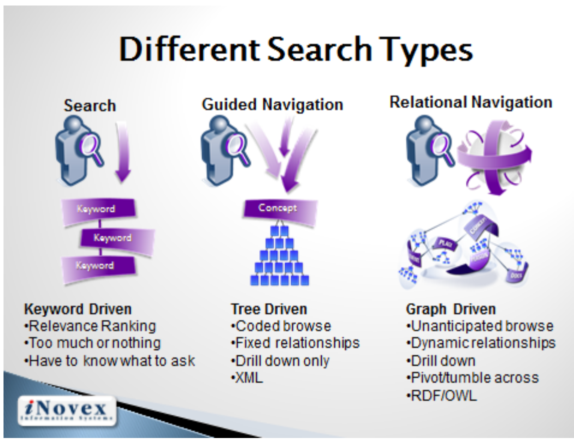
brief history of the semantic web was presented and started with a depiction of the web that most people see today: documents and web pages presented to the user through a web application. It then depicted a transition to an intermediate state where documents and data can co-exist on a semantic web riding atop the same infrastructure (http:). Even in this state, the data can be directly interpreted by a machine. The history concluded with a depiction of data being extracted from a document to become part of the web of data.

The basics of semantic technology were presented and emphasized that the technology has a foundation based o formal logic that enables software to understand information and reduce the need for a human to interpret the meaning. This section of the presentation concluded with a chart depicting how “triples” link to each other to form a web of data.

The final section touched upon adoption of and things to consider when semantic technologies are being considered as solution for community or enterprise.







Big Data and Semantic Technologies

Harlan Shober, RJ Lee Group

The presentation started with a description of entities that comprise laboratory informatics with the central elements being a federated architecture, scientific "Big Data" management and workflow-driven Laboratory Information Management Systems (LIMS). To aid attendee understanding, initial context was provided by first defining for "Big Data" and Semantic Technologies. Context was further bolstered through a description of a problem that included laboratory testing/characterization and fabrication processes. The challenges for a typical laboratory include the use of many systems and the creation of large amounts of data that grows daily but cannot be readily accessed.

After the context was established, the needed functionality was described and consisted of several elements: contribute, index, search, analyze, and archive. While bearing in mind the needed functionality, a string of universal scientific data management process categories were then presented with the intent of applying the universal description to the materials design and development domain.

Though semantic technologies are applicable over the entire lifecycle of the data management process, three categories were specifically identified as primary candidates for their application: Data Acquisition, Data Manipulation and Storage, and Discovery and Advisory. W3C standards for Resource Description Framework (RDF) were applied to a notional example with the intent of completing a thread that gave the attendee a sense of how this technology could be applied.

The presentation continued with a description of Postulate, a specific solution developed by RJ Lee Group that could be used as part of a suite of tools to enable the capture of data and the near-frictionless tagging of data with additional observations, provenance information, or links to additional data. Using tools like Postulate, repositories could be more easily shared with others in a federated manner. These technologies would enable the development of indices that increase the precision of search results and ease analytics since the data would be "self-described."

In the remainder of the presentation, Postulate functionality was further described, and some of the challenges presented earlier were addressed. For example, how do you process the quantity and variety of data, how do you store it, how do you find the data you care about, and how can the data be presented to you in a meaningful way?

Natural Language Processing (NLP)

Tim Hawes, Decisive Analytics

The presentation provided the attendees with a description of NLP and how it can be used. It started with examples of how it can be used to mine "Big Data" to predict credit card fraud or assess user purchase histories for product development. NLP is also being used in the field of biology and appears to have enjoyed some level of success.

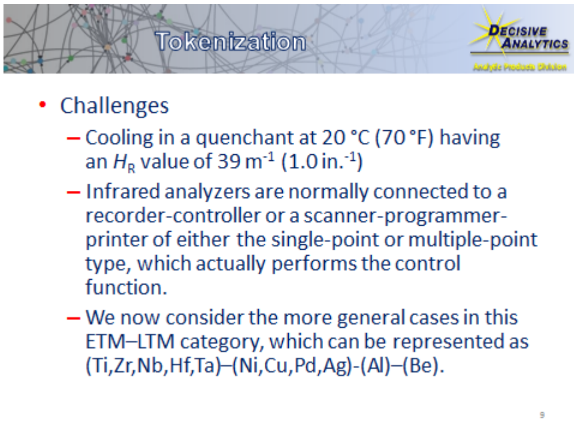
Since the biology and materials communities both publish large volume of documents (abstracts, papers, presentations, etc.), many of the NLP approaches developed for biology may be applicable to materials.

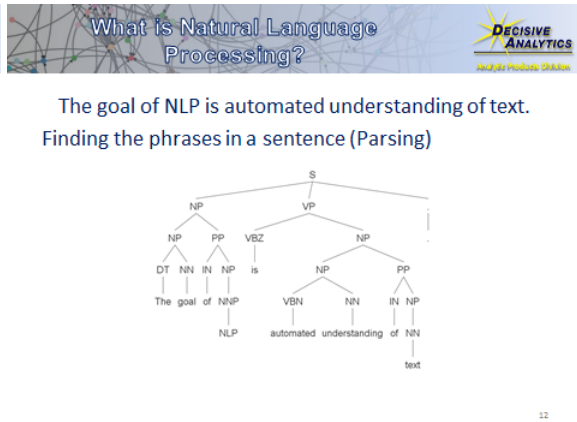
The next section of the presentation focused on describing various aspects of NLP: tokenization, part-of-speech tagging, disambiguation, parsing, entity disambiguation, and role labeling. This was helpful in removing the mystery surrounding NLP for those who hadn't had previous exposure.

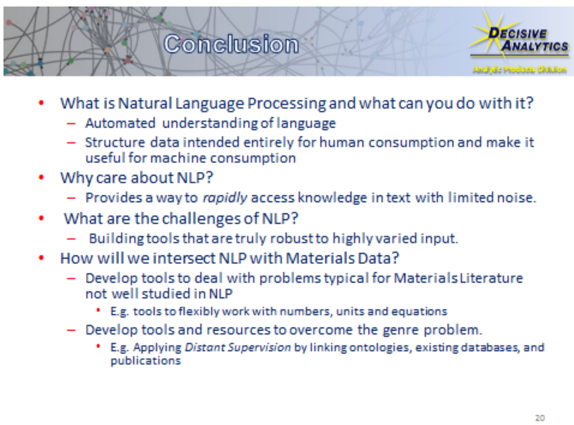
Typical products from NLP would be useful to the materials development community. Examples include providing the gist of a document's content, providing answers to natural language questions, and knowledge construction.

Specific NLP challenges for the materials domain were identified: inline use of equations, prevalence of tables, graphs and images (more of a computer vision problem) and numerically driven information. Additionally the "genre" problem was discussed as well as a way this might be addressed using raw data (versus learning data) and semi-supervised learning, active learning, and distant supervision approaches.

The presentation concluded by reiterating how NLP can be used and the value of using it, describing some its limitations, and identifying tool development needed for the materials domain.







Community and Government Priorities in Addressing Materials Data

The following numbered priorities for both community and government actions were 'rolled up' from workshop participants' inputs and were reviewed at the workshop. The raw inputs provided by participants are captured under each numbered priority and provide context to the priority and often more specific actions.

Community-Led Priorities

1. Develop and deploy standards for data and federated/collaborative environments

- Promote standards for data and collaboration environments
- Designing and deploying suitable software environments that are capable of facilitating, e-recording, and accelerating (fail often-fail fast) of the community's experience (both successes and failures) in exploring integrated workflows needed to realize the vision of ICME and MGI
- Data standards (program management/technical data/metadata)
- Community must start developing a common data format. data "package" could look like an HDF5 file and be shared in a variety of systems
- Begin definition of standardized infrastructure
- Produce draft guideline for the metadata including information regarding authorship, provenance, target…
- Share the data types being collected with the community. Include name/type/units of data
- Community must adopt a federated approach - allow organizations to autonomously create their own toolsets, but be able to read/write to the common data package mentioned in point 1.
- Good documentation on repositories are important
- Address networking of repositories (lightweight metadata database/index)
- Digital heterostructure microstructure mapping algorithms for both scanning electron microscopy (SEM) and transmission electron microscopy (TEM)
- Materials process model (thermodynamics) integration with ICMSE (Integrated Computational Materials Science and Engineering) data flow
- Data sharing protocol across users (government, OEM, developers) with appropriate security control
- Work with instrument/equipment OEMs to get auto ingest capabilities and open architectures
- Work together to define common vocabularies for interoperability
- Standard tests for ICME model data standards for microstructure data
- Standards for ICME model data storage and workflows

2. Communicate the value and need for digital materials data

- Brand management – consistent messaging of goals and beliefs
- Share success stories
- Value (ROI, Return on Investment) o data capture (globally, locally)
- Give incentive ($$$) for case studies to provide evidence that a shared data repository can be actually useful beyond the archival purpose

- Share ROIs for MII (the Materials Innovation Infrastructure)
- ICME projects, due to their iterative nature, take longer and are more expensive to realize benefits in industry implementation. Multi-year ICME programs are becoming a hard sell to management, difficult to establish ROI and realize benefits claimed.

3. Engage the community

- Write grant proposals
- Collaboration (or e-collaboration) science that will help us identify the specific incentives and impediments for establishing mutually beneficial, highly productive, sharing of expertise between disciplinary experts in materials, manufacturing, and data sciences
- Continue to work o hard problems—develop open source codes: discover new descriptors, data mining, uncertainty analysis
- Organize as a community (government/industry/academia, national/international)
- Follow data recommendations in MGI strategic plan—workshops to develop roadmap
- Attend more events like the MGI workshop — gaining lessons learned from other organizations is extremely valuable

4. "Define critical data" to be compiled

- Consensus o what fundamental genomic data is most-important to compile (thermodynamics? kinetics? properties [strength]? high-throughput DFT?)
- Agree to the concept of a "universal repository" for all genomic data that everyone will contribute to and use (cf. everyone maintaining and hosting their own databases); this includes issues of data security and sharing, etc.
- List of most-important ICME/MGI materials development activities, from an industry/commercial perspective (alloys? composites? piezoelectrics? etc.)
- Some ongoing repository efforts seem redundant. We should avoid unnecessary competition and try not to step o other people's toes.

5. Explore and leverage data solutions developed outside materials community

- Semantic web infrastructure – evaluate feasibility of 'unstructured materials data" management (Technical path/cost/timeframe)
- Keep communicating outside the community about solutions
- Focus on available tools, open ones when possible

6. Train students

- Sponsor students who can think in terms of IT and MSE
- Training workshops (through professional societies) for training the new generation of materials students and researchers in the use of readily (already) accessible data science tools and cloud services to make the best use of this emerging infrastructure in enhancing their own individual day-to-day productivity.

7. Establish community norms for publishing materials data

- Involve publishers by requiring data when publishing. Begin by making just the data available first and then work on standardization panel

- Data associated with publications should be shared along with the publications. Not only the metadata (e.g. average grain size vs cooling rate) but also the source of the data (e.g. micrographs used to generate grain size, temperature/time charts used to calculate cooling rates, etc.)

Government-Led Priorities

1. Lead data strategy/approach development

- Hold meeting like this one in 6-12 months with purpose of developing roadmap for MII
- Define a technical roadmap for the materials data infrastructure
- Government's got to decide on a strategy
- What's the critical nucleus? e.g., getting CALPHAD off the ground
- Government must establish an official stance on security and infrastructure.
- List of most-important ICME/MGI materials development activities, from a government perspective (alloys? composites? piezoelectrics? etc.)
- Needs assessment for professional workforce development
- Work with industry to make sure the research-to-engineering gap is filled. What is the practical use of the projects
- Provide the materials community organizing function
- Business case for productivity improvement with data readily available
- Facilitator as honest broker of capability awareness and data sharing
- Interdisciplinary coordinated effort to avoid/minimize duplication and redundancy

2. Facilitate data deposition (policy & technology)

- Setting expectations and guidelines for best practices and standards, where relevant
- Invest in tool making data management as easy as possible
- Promote standards development/common data structures/share knowledge representations
- Learn about the WBC Semantic Web capabilities, and limitations
- Government should foster community development for both data package refinement and creating standard approach to creating an enterprise toolset.
- Provide motivation for standard data collection; ensure it includes pedigree/provenance/meta-data
- Facilitator for materials data standards (good and trustworthy data vs. bad data)
- Facilitator for forming consortium for data mining, data warehousing, and sharing
- Facilitate industry standards for ICME model validation and maturity levels
- Facilitate standards for model-based process and supplier qualification

3. Incentivize data deposition

- Provide motivation for standard data collection, ensure it includes pedigree/provenance/meta-data
- Push "data management plan" requirements to "data deposit" requirements
- Make data sharing a requirement
- Contractual requirements that preserve data for future use
- Demand data submission as a deliverable that will be in the contract before paying the funds.
- Require that any data generated by federal grants is provided to the government (or a designated repository) within 3 years after completion—start with basic research
- Demonstrate the return on investments in the materials data infrastructure

4. Support data sharing and deposition (provide resources)

- Increase % of MGI funds dedicated to MII development to 10%--repositories & collab. platforms
- Commit to long-term support for data repositories & collaborative platforms
- Funding for development / collection of fundamental genomic data
- Support thermodynamics/kinetics database development for light-weight alloy systems
- Funding for universal data repository (e.g., at NIST) – creation and maintenance
- Fund or establish data repositories with common/uniform data collection format
- Create/identify secure data sharing site (like AMRDEC) for government contractors—not a repository
- AFRL take lead o making a database that can be shared
- Infrastructure for materials related semantic web applications

5. Support data creation

- Support experimental measurement effort to provide quality data for database development
- Support more high-throughput (HT) studies for applied programs to populate data. Current HT approaches support are limited to 'too' fundamental single-phase DFT calculations

6. Enhance data management competency

- Government needs to increase in-house expertise in these areas, or alternatively, work closer with groups like NIST. We cannot allow other organizations to define our needs for us.

7. Provide quality datasets for model development/validation

- Need for open model benchmark cases with data to be available to the community.

Attendees

John Allison	University of Michigan
John Beatty	Army Research Laboratory
Ben Blaiszik	University of Chicago/ANL
Carrie Campbell	NIST
Sam Chance	Inovex
Jennifer Fielding	Air Force Research Lab
Marco Fornari	Central Michigan
Tim Hawes	Decisive Analytics Corp
Lou Hector	General Motors
Andrea Helbach	Air Force Research Lab
Kris Hill	ITI-Global
Mike Glavicic	Rolls Royce
Ro Gorham	NCDMM
Dennis Griffin	NASA
Mike Groeber	Air Force Research Lab
Scott Henry	ASM International
Matt Jacobsen	Air Force Research Lab
Will Joost	Dept of Energy-EERE
Surya Kalidindi	Georgia Tech
Kevin Kendig	Air Force Research Lab
Ben Leever	Air Force Research Lab
Lara Liou	GE Aviation
Kenny Lipkowitz	Office of Naval Research
Bill Mullins	Office of Naval Research
Benji Maruyama	Air Force Research Lab
Rajiv Naik	Pratt & Whitney
Jim Neumann	Honeywell
Ruth Pachter	Air Force Research Lab
Clare Paul	Air Force Research Lab
Amra Peles	United Technologies Research Center
Andy Powell	GE Aviation
Brian Puchala	University Michigan
Ajit Roy	Air Force Research Lab
Ayman Salem	Materials Resources
Tom Searles	Materials Data Management
Jason Sebastian	Questek
Richard Serwecki	NASA
Dongwon Shin	Oak Ridge National Labo

Harlan Shober	RJ Lee
Jeff Sheehy	NASA
Jeff Simmons	Air Force Research Lab
Veera Sundararaghavan	University of Michigan
Sesh Tamirisakandala	RTI
Glenn Tarcea	University of Michigan
TJ Turner	Air Force Research Lab
Vasisht Venkatesh	Pratt & Whitney
Chuck Ward	Air Force Research Lab
Jim Warren	Natl Institute of Standards & Tech
Jeff Williams	GE Aviation
Terry Wong	Rockedyne
Wayne Ziegler	Army Research Laboratory
Jake Zindel	Ford Motor Company