NIST and The Materials Genome Initiative

Some Highlights and Topics for the PCO

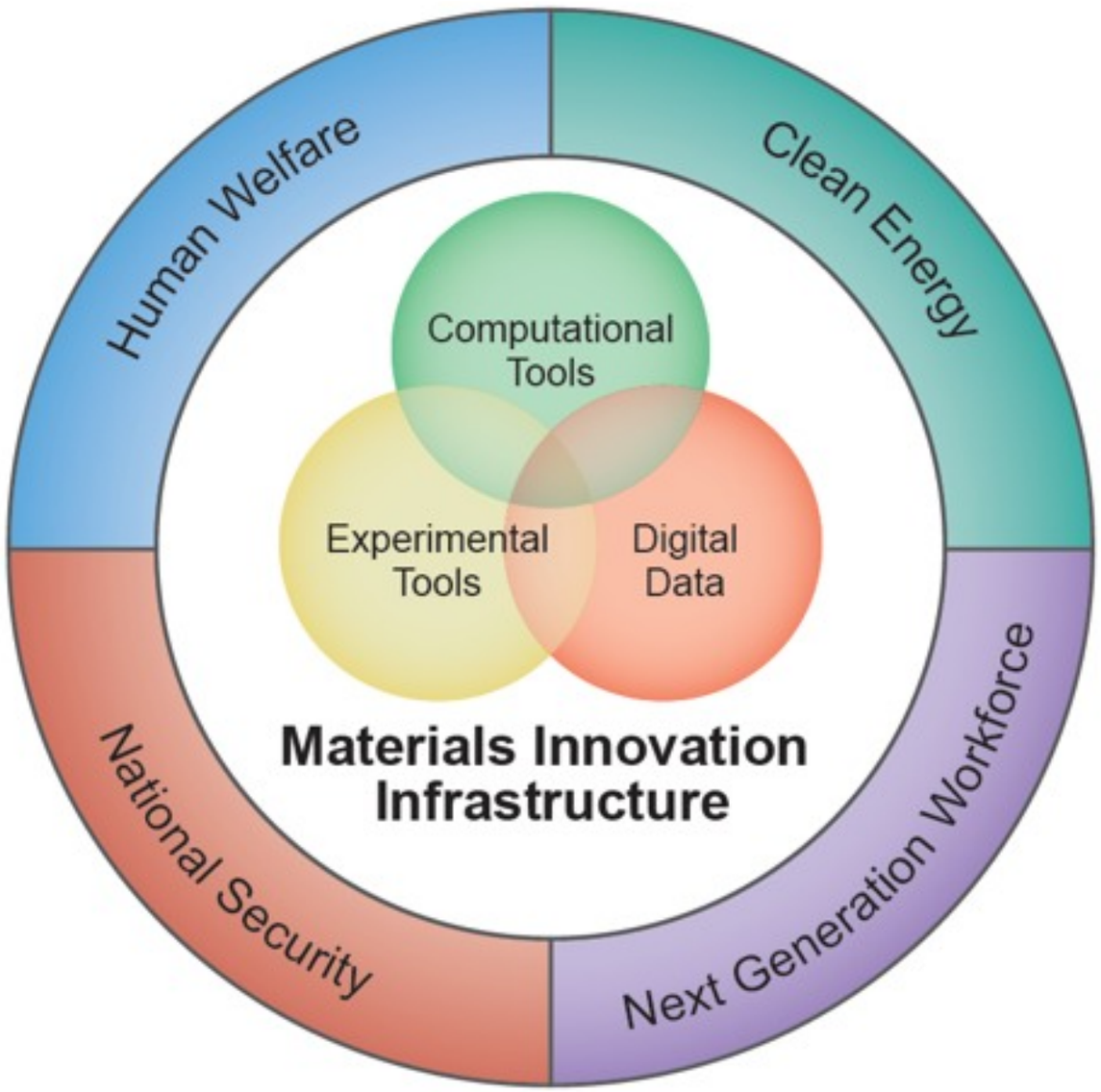
Material Measurement Laboratory

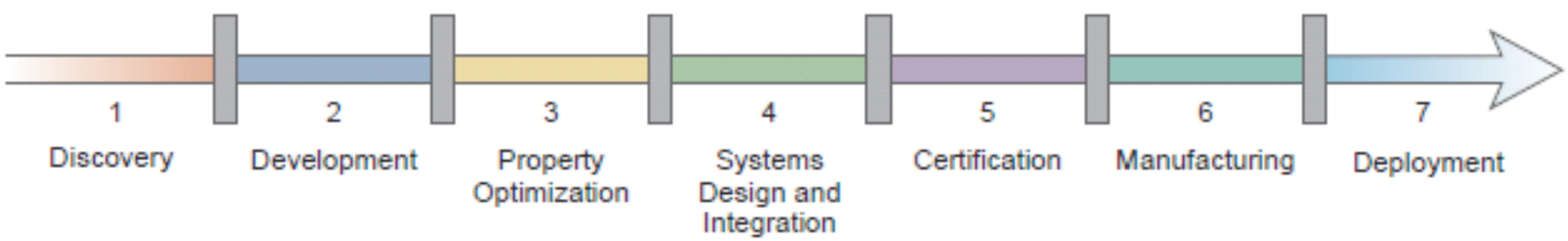
National Institute of Standards and Technology

The Materials Genome Initiative (MGI)

Goal:
To decrease the time-to-market for new materials by >50%.

The Materials Innovation Infrastructure





NIST and MGI

2010 2011 2012 2013

NIST, DOE, NSF, and DOD work with OSTP to prepare MGI White paper

NIST develops Initiative, $4M allocated for internal programs

04/12: NSTC Subcommittee (CoT) on the Materials Genome Initiative formed (NIST, DOE, DOD, NSF, NASA, NIH, USGS, NNSA, DARPA, NSA, OMB)

6/12: MGI White House Kickoff Event www.whitehouse.gov/mgi

2/13:
•Subcommittee co-chairs announced -L. Locascio (NIST), H. Kung (DOE)
•Strategic planning kicked off
•Focus teams formed: Data, Code Curation, Industry Outreach, Transformational Challenges
•Draft SP for 2 year Anniversary

Federal Programs

The federal government has announced several programs and funding opportunities related to the Materials Genome Initiative. Learn more about these activities below:

Federal Funding Announcements

FY 2012

Department of Energy:

- Funding announcement for the development of lightweight materials and awardees.
- Funding announcement for predictive theory and modeling for advanced materials.
- Funding announcement for Scientific Discovery through Advanced Computing (SciDAC) partnerships.

Department of Defense:

- Funding announcement for the Enterprise for Multiscale Research of Materials program, led by the Army Research Laboratory (ARL).
- Funding announcement for the Air Force Research Laboratory (AFRL) Center of Excellence for Integrated Computational Material Science and Engineering of Structural Materials
- Funding announcement for the Air Force Research Lab (AFRL) Center of Excellence in advanced organic composites
- Beta release of the Ab-Initio Electronic Structure Library (AFLOWLIB), maintained by Duke University in partnership with the Office of Naval Research, with open access to over 17,000 compounds derived from the Inorganic Crystal Structure Database and over 160,000 binary alloys

National Institute of Standards and Technology:

- Funding announcement for the NIST Advanced Materials for Industry program.

National Science Foundation:

- Funding announcement for the FY 2012 NSF Designing Materials to Revolutionize and Engineer our Future (DMREF) program.

NIST Supports New Collaboration Modalities

NIST, industry and the MGI

- June 25-26, 2013 Grand Challenges Summit to seek stakeholder input on critical industrial problems that MGI should target

- NIST-DOE Sponsor

- 50/50 Industry/Academia (plus the usual cohort of USG)

- Output to inform Strategic Plan

EERE Collaboration

U.S. Department of Energy

Office of Energy Efficiency and Renewable Energy

Fiscal Year 2013 Vehicle Technologies Program

Wide Funding Opportunity Announcement

Funding Opportunity Announcement (FOA) Number: DE-FOA-0000793
FOA Type: FINAL
CFDA Number: 81.086

Dissemination of Data and Results

In support of the President's Materials Genome Initiative, and to ensure that the results supported by this AOI can make the broadest impact, awardees are required to disseminate the results of **their work through infrastructure and methods identified by the National Institute of Standards and Technology (NIST)**. NIST will provide data schemas and informatics tools in accordance with the specific data types generated by the project; for example tracer, intrinsic and chemical diffusivity data; diffusion couple data; and phase transformation data from differential scanning calorimetry, differential thermal analysis, continuous cooling transformation data, and isothermal cooling transformation data. In addition to the specific tools for kinetic data, a variety of other data platforms will be offered. Specific file repositories will be provided for CALPHAD assessment files, first-principles files, and interatomic potentials (*http://www.ctcms.nist.gov/potentials/*). In addition to these specific file repositories, a general file repository platform will be established for all other data, which cannot be captured by the previously mentioned tools. In addition, dissemination of results via publication in peer-reviewed journals will be encouraged. Additionally, applications must describe how such data will be valuable in the development of high performance magnesium casting alloys

NIST Coordinates New Approaches

- Ideation Challenge on Materials Data Infrastructure (collaboration with AFRL)

- Draft text:

  To respond to this ideation challenge, please describe the necessary ecosystem and estimate the costs to be incurred to establish, operate and maintain the hardware, software, and personnel needed to house and serve this data in a manner that is

  - Cost efficient
  - Enables rapid web-based discovery and retrieval of information
  - Ensures that the data retrieval has both high precision and recall.
  - Scalable
  - Standards-based

What is the End State?

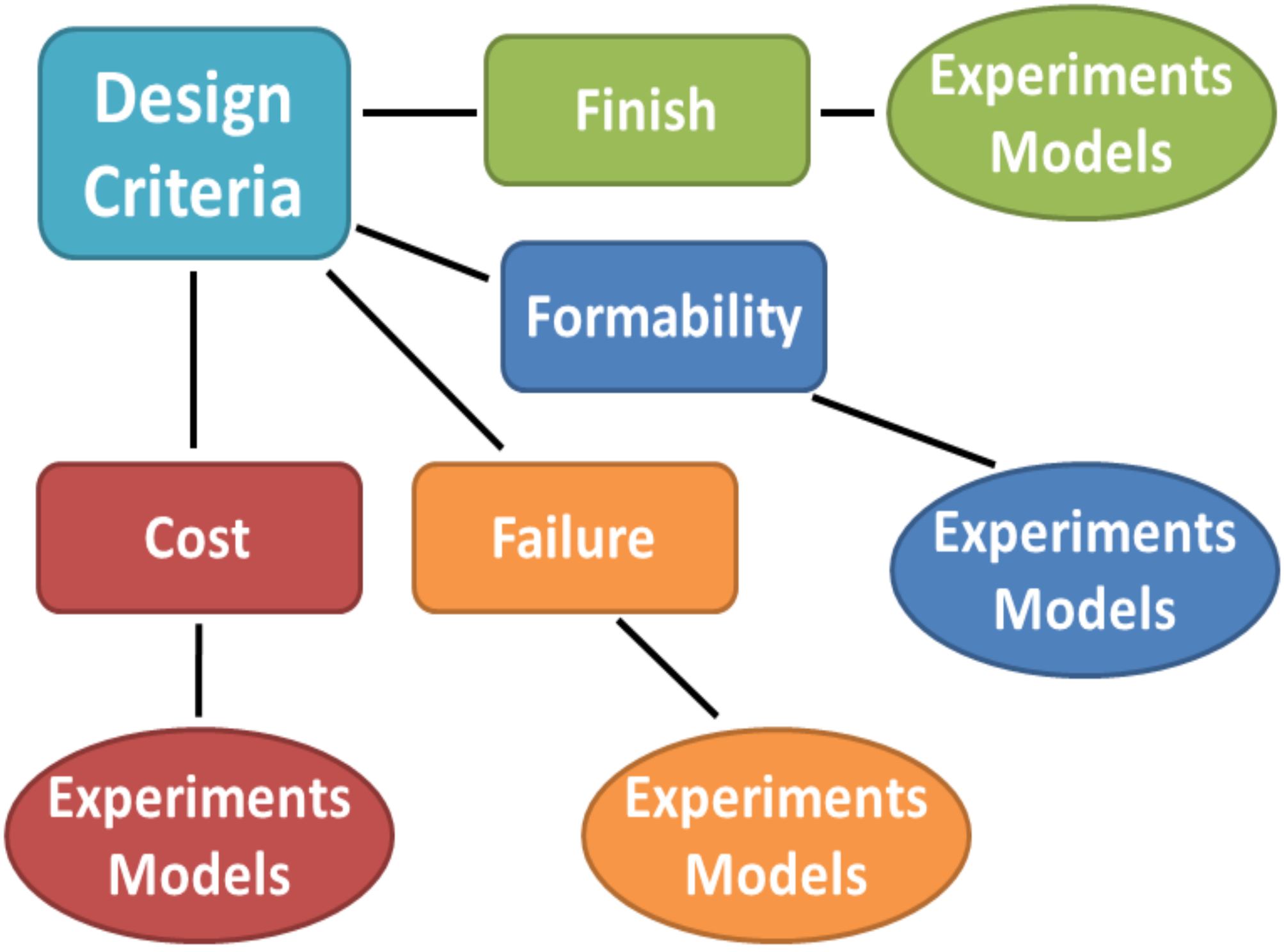


Figure 1. Schematic of how the design criteria for a given material dictate the needed material properties and thus define the needed experiments, models and data.

A Useful Conversation

- Major Programmatic Refactor underway

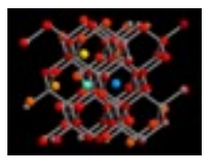
Data

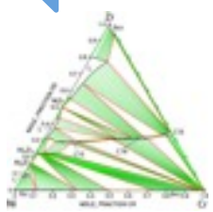
Models

$A = \pi r^2$

Today's Approach to Computational Materials Design

Experiment




Quantum Nano Micro Macro

Simulation

Materials

w/ Targeted Properties

Data

Repositories

Simulations

Experiments

Data

Models

Code

Metadata

Models

$A = \pi r^2$

MGI

How do we do it?

Experiment

Quantum

Nano

Micro

Macro

Simulation

Materials

w/ Targeted Properties

Data

Models

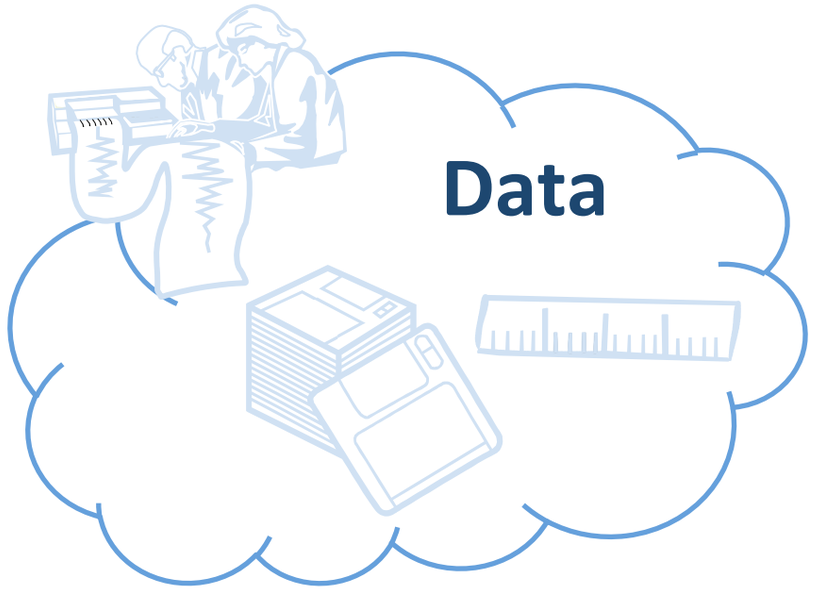
$A = \pi r^2$

Community-based
Curated Repositories

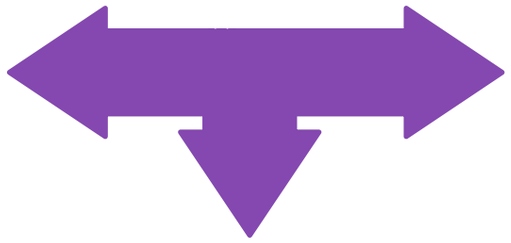
MGI

Ecosystems

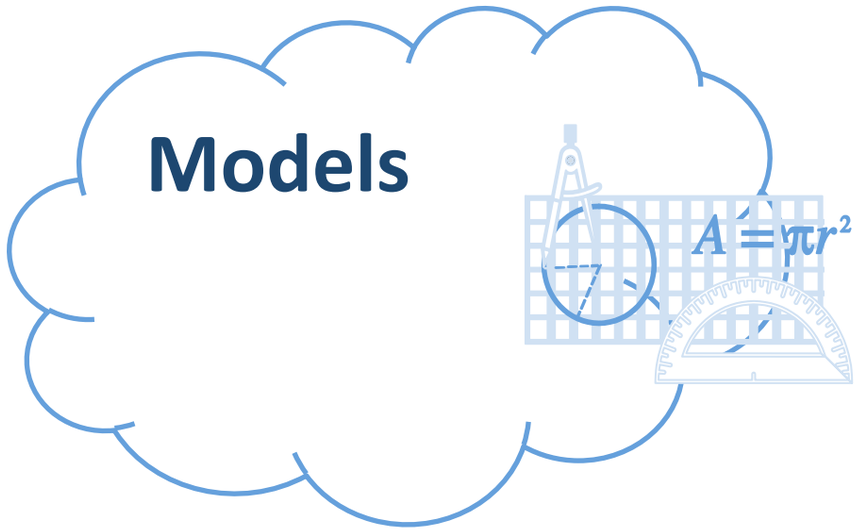
Materials w/ Targeted Properties



Data



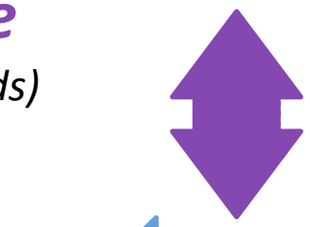
Repositories



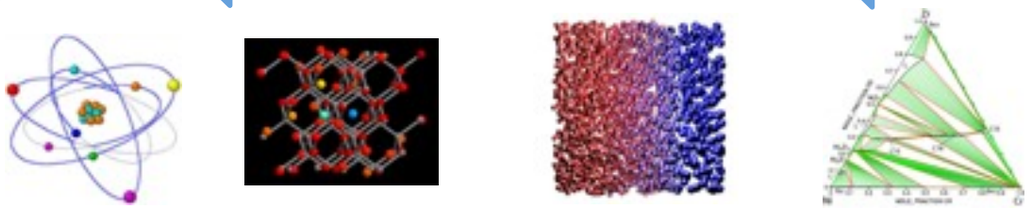
NIST

*Enable & Enhance **Exchange***

(repositories, disciplines, industries; standards)



Experiment



Quantum **Nano** **Micro** **Macro**

Simulation

Materials w/ Targeted Properties

Data

Repositories

Simulations

Experiments

Data

Models

Code

Metadata

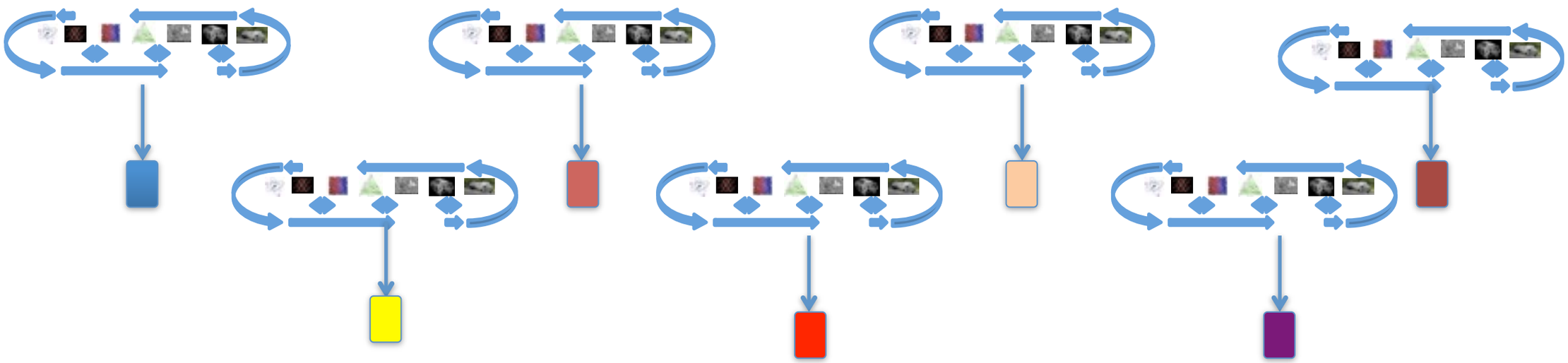
Models

$A = \pi r^2$

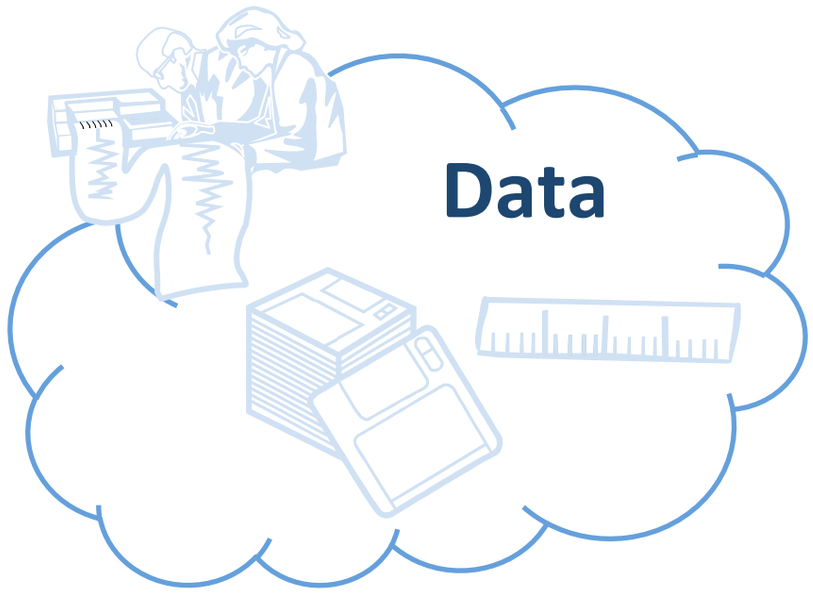
NIST

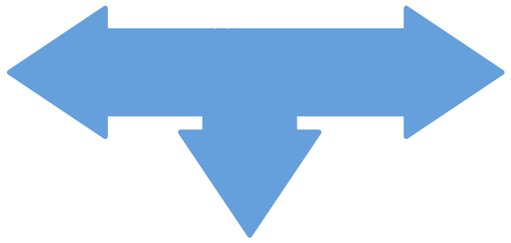
*Assess & Improve **Quality***

(Data & Models)

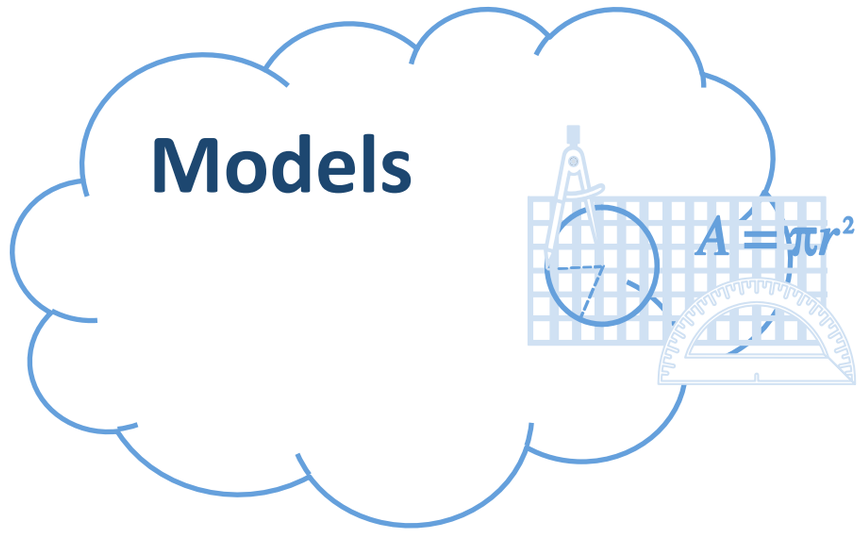


Materials w/ Targeted Properties





Repositories



NIST

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(repositories, disciplines, industries; standards)

NIST

*Assess & Improve **Quality***

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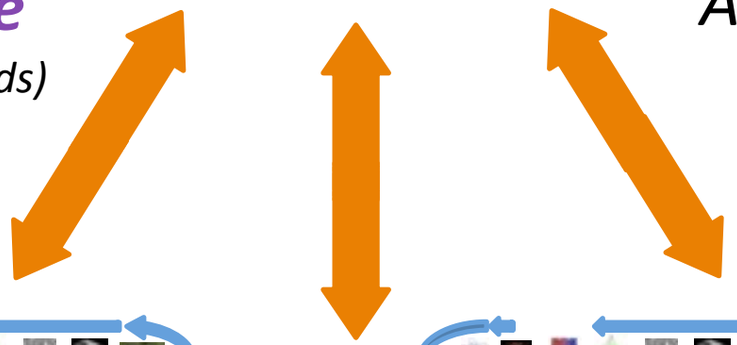
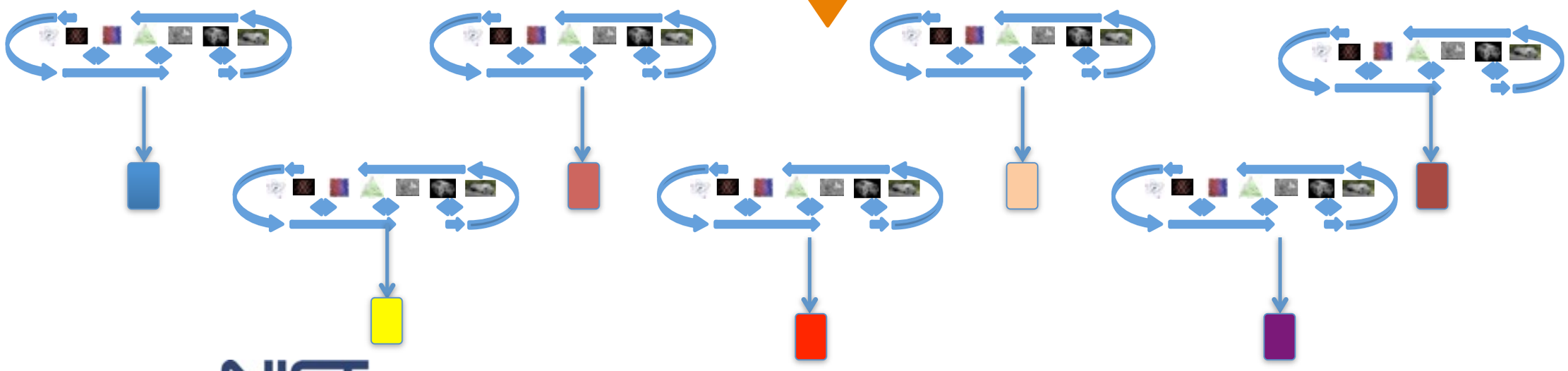




NIST

*New **Methods and Metrologies***

(data driven analysis and models)

Materials w/ Targeted Properties

Short Summary

To foster widespread adoption of the MGI Paradigm both across and within the multitude of materials development ecosystems

NIST is establishing essential data exchange protocols and the means to ensure the quality of materials data and models

Yields new methods, metrologies and capabilities necessary for accelerated materials development.

*Enable & Enhance **Exchange***

- Develop and deploy repositories
- Develop and disseminate materials informatics infrastructure
  - Enable data discovery through tools and standards
  - Capture data from scientific workflows and archival sources
  - Engage with stakeholders to determine needs and disseminate best practices
- Integrate across length and time scale
- Build and Test infrastructure through Pilots

Assess & Improve ***Quality***

- Validate Experiments and Models
- Verify Model accuracy
- Quantify Uncertainty
- Quantify Sensitivity
- Define Next Generation of Experiments and Models

*New **Methods and Metrologies***

- Develop Data Driven Materials Science
- Integrate with Modeling Expertise
- Achieve targets in Materials by Design/ICME

New White House Push

EXECUTIVE OFFICE OF THE PRESIDENT
OFFICE OF SCIENCE AND TECHNOLOGY POLICY
WASHINGTON, D.C. 20502

February 22, 2013

MEMORANDUM FOR THE HEADS OF EXECUTIVE DEPARTMENTS AND AGENCIES

FROM: John P. Holdren
Director

SUBJECT: Increasing Access to the Results of Federally Funded Scientific Research

1. Policy Principles

The Administration is committed to ensuring that, to the greatest extent and with the fewest constraints possible and consistent with law and the objectives set out below, the direct results of federally funded scientific research are made available to and useful for the public, industry, and the scientific community. Such results include peer-reviewed publications and digital data.

http://whitehouse.gov/sites/default/files/microsites/ostp/ostp_public_access_memo_2013.pdf

Office of Data and Informatics

SRD

- continue existing SRD distribution
- Quality Framework
- SRD Modes
- assess external need
- new product ideas
  - SRMDS
  - data streams
  - alternative delivery methods
- Open Data Initiative
- Open Govt Directive
- Data.gov

Research Data

- deal w/ data deluge
- provide advice to MML bench staff
- gather best practices
- interpret external rules & regulations
- reduce redundancy
- promote cooperation and coherent action
- manage changes in scholarly publishing
- coordinate with
  - WERB
  - Library
  - JResNIST

Lead/Liaison

- partner with ITL
- represent MML
  - NIST committees
  - NSTC & IWGs
  - NIH, NSF, DOE
  - other Fed Govt
  - Research Data Alliance (RDA)
- data standards
- champion proposals
  - budget initiatives
  - IMS
  - inter-agency, RDA

Data Science

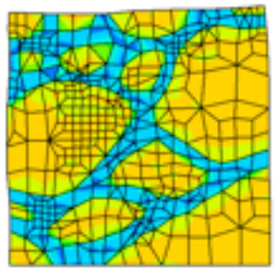
The 4th paradigm?

- will it stand next to
  - theoretical
  - experimental
  - computational
- Cloud
- Statistical Learning
- Big Data
- Knowledge Discovery
- very fast growing
- *many* new jobs
- new degrees/depts

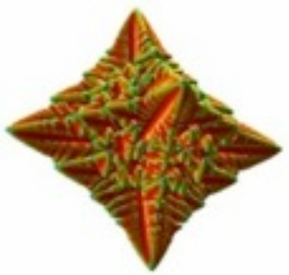
Structural Alloys Pilot

Macroscopic Materials Properties

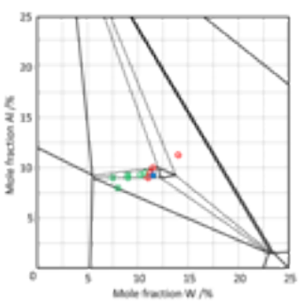
MATERIAL PROPERTIES



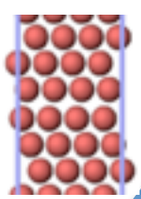
Structure-Property Relationships
Computation, Theory, Expt

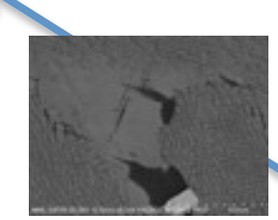


Processing-Structure Relationships
Phase-field, FE, etc.



Composition Dependent Databases
CALPHAD, Diffusion Mobility





Collaborations
Universities
Industry
MML (3 Divisions)
ITL

Crosscuts
Repositories
Workflow Tools
Standards
Protocols
Uncertainty
Dissemination

Atomic Structure and Properties

Atomic Scale Models
Ab initio, Molecular Dynamics, Monte Carlo, Embedded Atom

Experimental Inputs
Crystal Structure, Diffusion, Thermochemical Data

Short Term Deliverables

- www.nist.gov/MGI
  - includes timeline and rollout data
  - existing resources and plans for improvements
  - current efforts of relevance
- Instantiation of a MGI file repository (3 months)
- Incorporation of MGI effort within NIST roll-out in response to Holdren Memo
- Specification of EERE deposition plans, invite participants to field test repositories
- Implementation of Thermodynamic Research Center model for data capture from the literature for phase-based data.
- Direct Collaboration/Mission Alignment with New ODI
- MGIDATA Communities initiated with populations driven from Grand Challenge workshop (leaders must be identified, and incentivized)
  - Pre-nucleate some communities
  - A great deal of effort should go in this area
  - Standards as output
- Outreach to Lightweighting community
- Outreach to Diffusion and Calphad communities
- Partnerships with ASM, TMS, KSU and GaTech pursued, and funded if deemed appropriate (others too?)