The Materials Genome Initiative, Data, Open Science, and NIST

James A Warren

Director, Materials Genome Program

Material Measurement Laboratory

National Institute of Standards and Technology

Executive Secretary, NSTC Subcommittee on MGI

Science advances one funeral at a time -Max Planck

The Perfect is the Enemy of the Good -Voltaire

The Materials Genome Initiative: A National Priority

"To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call the Materials Genome Initiative.

The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place.

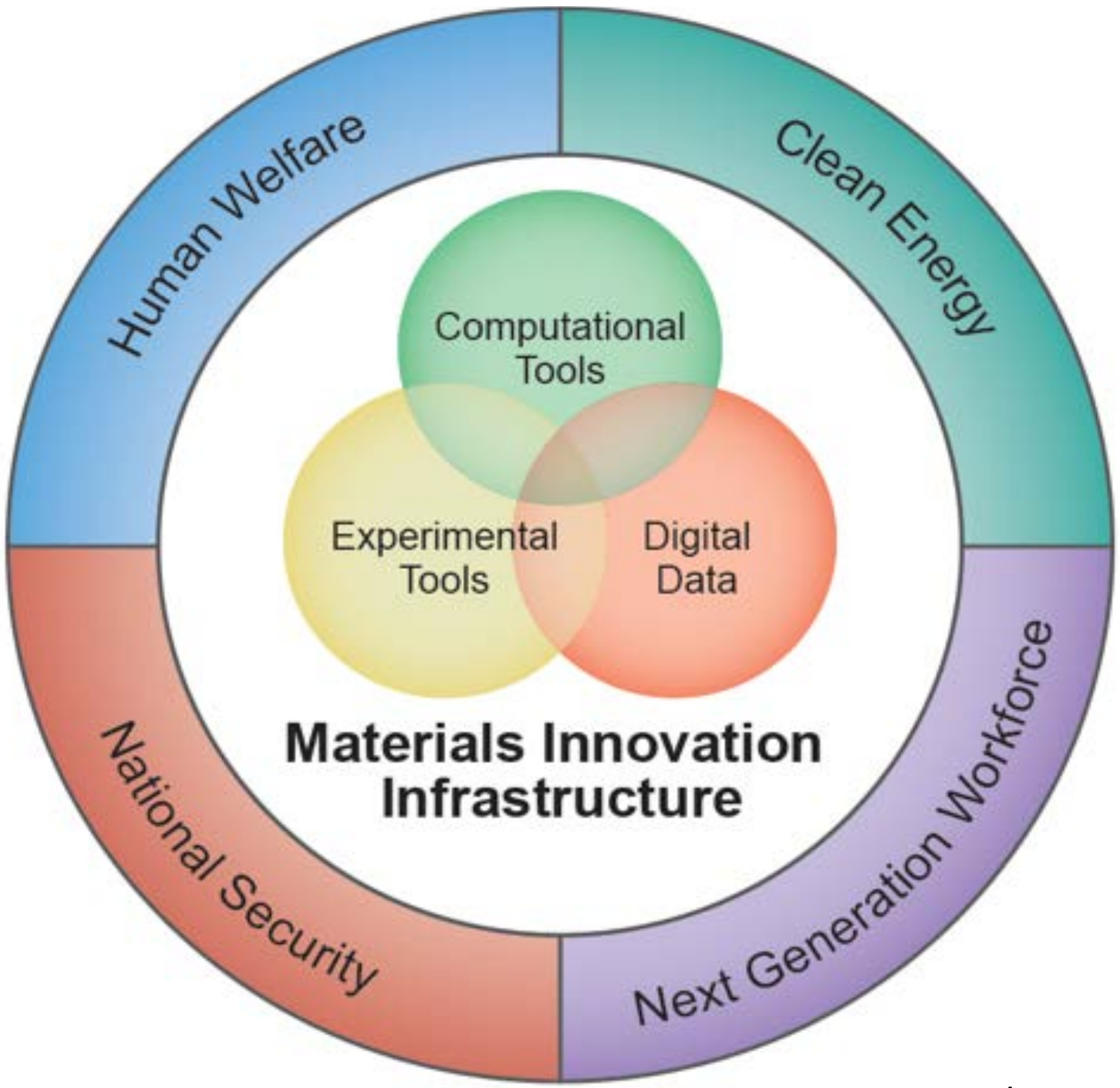
We can do it faster."

-President Obama (6/11)

There are two groups of people that don't like the name Materials Genome Initiative

THE MATERIALS GENOME INITIATIVE

to decrease time-to-market by 50% while <$$



Develop a Materials Innovation Infrastructure

Achieve National goals in energy, security, and human welfare with advanced materials

Equip the next generation materials workforce

Materials Genome Initiative for Global Competitiveness

A Multi-Agency Effort

The MGI Subcommittee (SMGI)

who we are

- MGI Subcommittee, Committee on Technology, NSTC
- First meeting April, 2012
- Membership includes the Federal agencies: NIST, DOE, DOD, NSF, NASA, NIH, US Geological Survey, National Nuclear Security Administration, DARPA, and Office of Management and Budget
- Co-chairs: OSTP (Whitman), AFRL (Ward), DOE (Horton)
- Executive Secretary: NIST (Jim Warren)

what we do

- Coordinate across government
- Convene stakeholders to engage in strategy: Grand Challenge Summits
- Development of a National Strategy for MGI

SIGN UP FOR OUR STAKEHOLDER EMAIL LIST!

www.mgi.gov

MGI National Strategy: 4 Goals

- Enable a Paradigm Shift in Culture
- Integrate Experiments, Computation, Theory
- Facilitate Access to Materials Data
- Equip the Next-Generation Materials Workforce

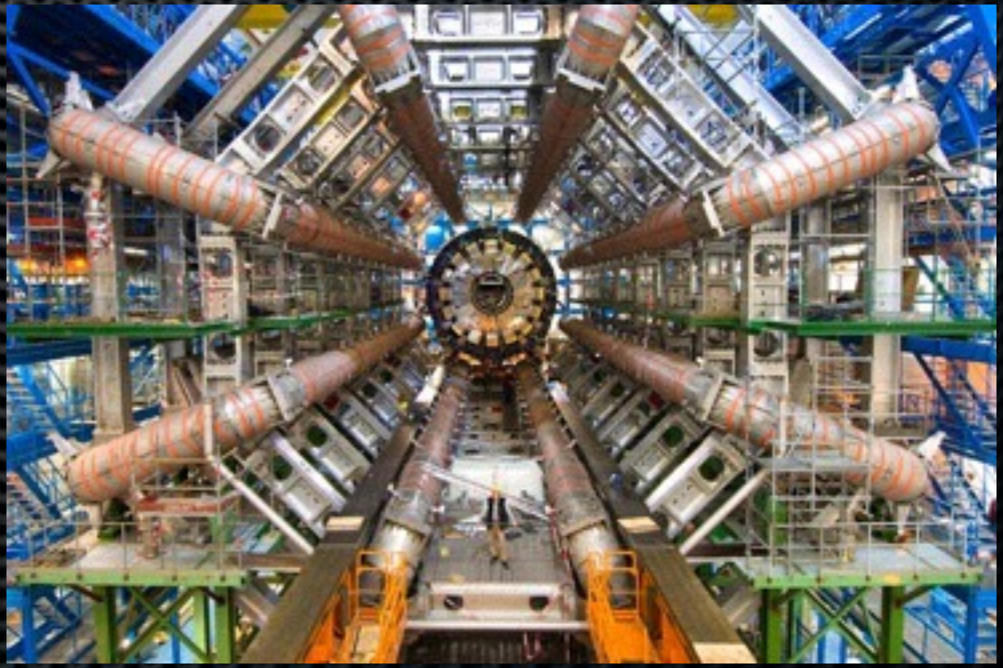
https://www.whitehouse.gov/sites/default/files/microsites/ostp/NSTC/mgi_strategic_plan_-_dec_2014.pdf

The Relationship between Models, Measurement, Data, and Publication

A simple example to illustrate the key questions, gaps, obstacles to realizing materials by design

Better Models = Less Data

- Take the LHC as an example
- Data produced at 1PB/sec !
- Reduced data saved: 300 MB/s
- That's a darn good model
- Other end : Biology?
- Materials: In the middle



- But you need to know the model to make sense of the data!

What should we be doing?

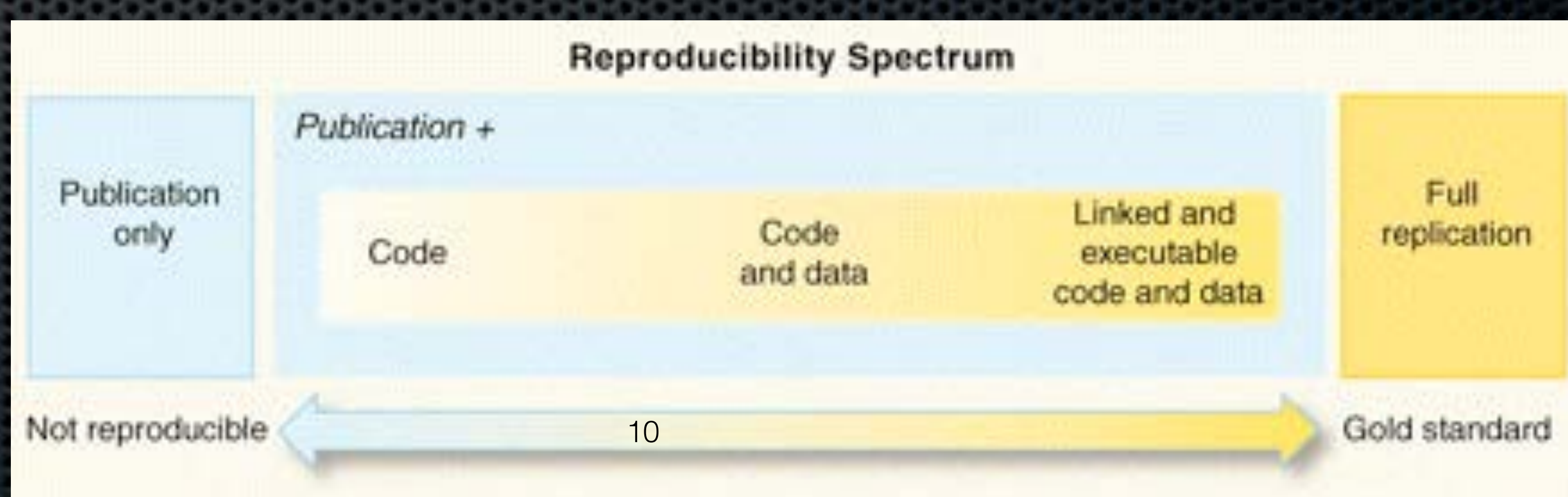
Science is characterized by the iteration of experiment and models, yielding higher fidelity with lower uncertainty.

The measurement or computation of a quantity (data) is generally *meaningless* without the associated quantifying model that defines both the data and its uncertainties.

Thus dissemination of data is ideally **the dissemination of the following information:**
1. **Measured quantities,**
2. **Associated quantifying models, and**
3. ***Raw data, including the protocols (and equipment) by which it was obtained***

PUBLISHING

see R. Peng *Science* 2 December 2011: 1226-1227



Consequences of the traditional approach

- High barrier to adoption of methods and results
- Extra expense due to duplication of effort
- Lost opportunities to enable discovery & further science

So Now What?

Formulating the NIST Role in MGI

Some background and further thoughts

NIST Products and Services

© Robert Rathe

Measurement Research

- ~ 2,200 publications per year

Standard Reference Data

- ~ 100 different types
- ~ 6,000 units sold per year
- ~ 226 million data downloads per year

Standard Reference Materials

- ~ 1,300 products available
- ~ 30,000 units sold per year

Calibration Tests

- ~ 18,000 tests per year

Laboratory Accreditation

- ~ 800 accreditations of testing and calibration laboratories

Data mandates in the Federal Government

OSTP "Public Access" Memo Feb 22, 2013

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 t... Research

OMB "Open Data" Memo May 9, 2013

EXECUTIVE OFFICE OF THE PRESIDENT
OFFICE OF MANAGEMENT AND BUDGET
WASHINGTON, D.C. 20503

THE DIRECTOR

May 9, 2013

M-13-13

MEMORANDUM FO... ENCIES

FROM: Sylvia M...

Executive Order May 9, 2013

For Immediate Release | May 09, 2013

Executive Order -- Making Open and Machine Readable the New Default for Government Information

EXECUTIVE ORDER

MAKING OPEN AND MACHINE READABLE THE NEW DEFAULT FOR GOVERNMENT INFORMATION

By the authority vested in me as President by the Constitution and the laws of the United States of America, it is hereby ordered as follows:

Section 1. General Principles. Openness in government strengthens our democracy, promotes the delivery of efficient and effective services to the public, and contributes to economic growth. As one vital benefit of open government, making information resources easy to find, accessible, and usable can fuel entrepreneurship, innovation, and scientific discovery that improves Americans' lives and contributes significantly to job creation.

Decades ago, the U.S. Government made both weather data and the Global Positioning System freely available. Since that time, American entrepreneurs and innovators have utilized these resources to create navigation systems, weather newscasts and warning systems, location-based applications, precision farming tools, and much more, improving Americans' lives in countless ways and leading to economic growth and job creation. In recent years, thousands of Government data resources across fields such as health and medicine, education, energy, public safety, global development, and finance have been posted in machine-readable form for free public use on Data.gov. Entrepreneurs and innovators have continued to develop a vast range of useful new products and businesses using these public information resources, creating good jobs in the process.

DATA Act, P.L. 113-101 May 9, 2014

S.994

One Hundred Thirteenth Congress of the United States of America

AT THE SECOND SESSION

Begun and held at the City of Washington on Friday, the third day of January, two thousand and fourteen

An Act

To expand the Federal Funding Accountability and Transparency Act of 2006 to increase accountability and transparency in Federal spending, and for other purposes.

Be it enacted by the Senate and House of Representatives of the United States of America in Congress assembled,

SECTION 1. SHORT TITLE.

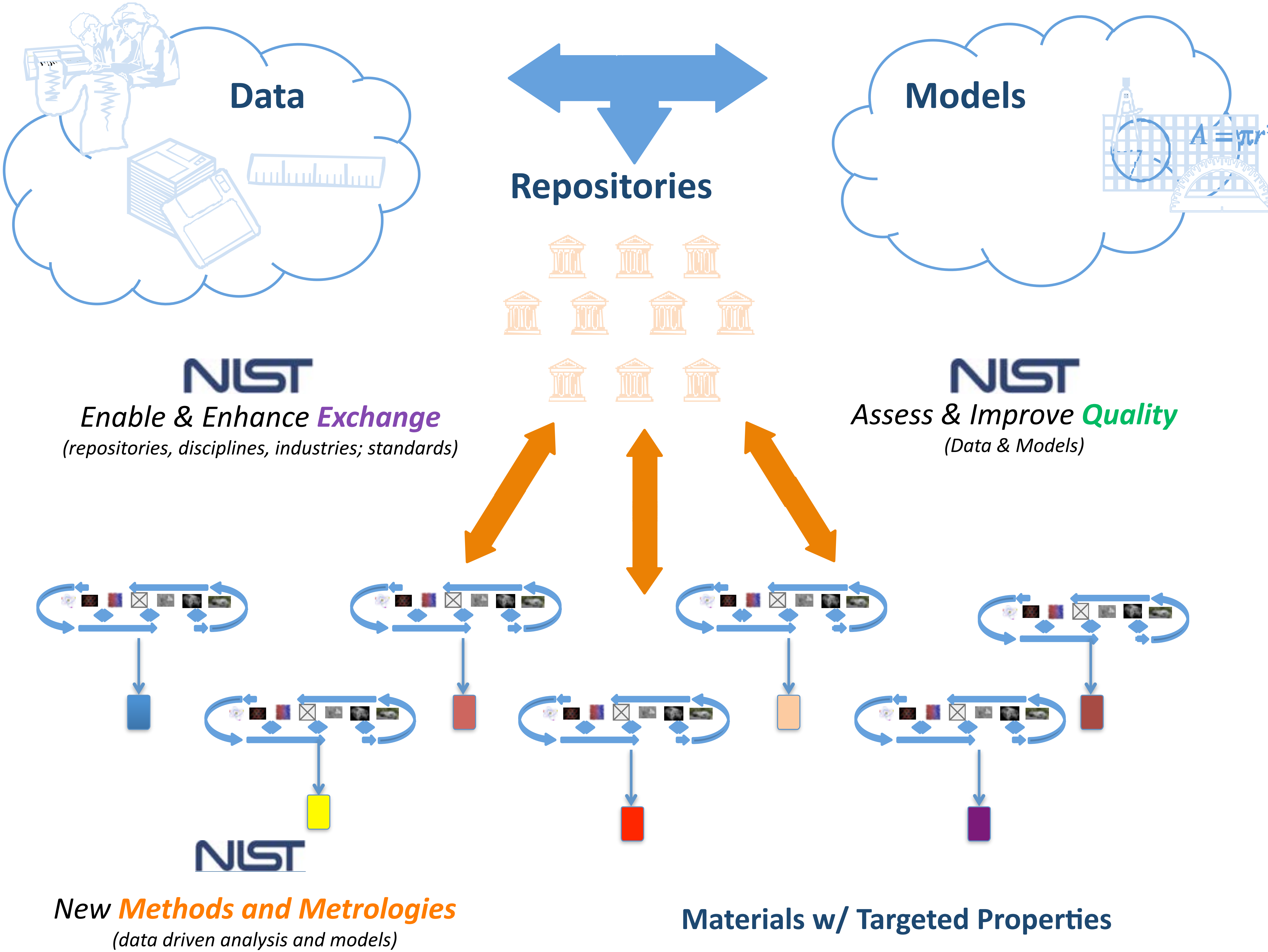
This Act may be cited as the "Digital Accountability and Transparency Act of 2014" or the "DATA Act".

SEC. 2. PURPOSES.

The purposes of this Act are to—

(1) expand the Federal Funding Accountability and Transparency Act of 2006 (31 U.S.C. 6101 note) by disclosing direct Federal agency expenditures and linking Federal contract, loan, and grant spending information to programs of Federal agencies to enable taxpayers and policy makers to track Federal spending more effectively;

(2) establish Government-wide data standards for financial data and provide consistent, reliable, and searchable Govern-


Data
Repositories
Models
$A = \pi r^2$
NIST
Enable & Enhance Exchange
(repositories, disciplines, industries; standards)
NIST
Assess & Improve Quality
(Data & Models)
NIST
New Methods and Metrologies
(data driven analysis and models)
Materials w/ Targeted Properties

SCOPE: Goals of Initiative

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

Goal 1: NIST establishes *essential materials data and model exchange protocols*

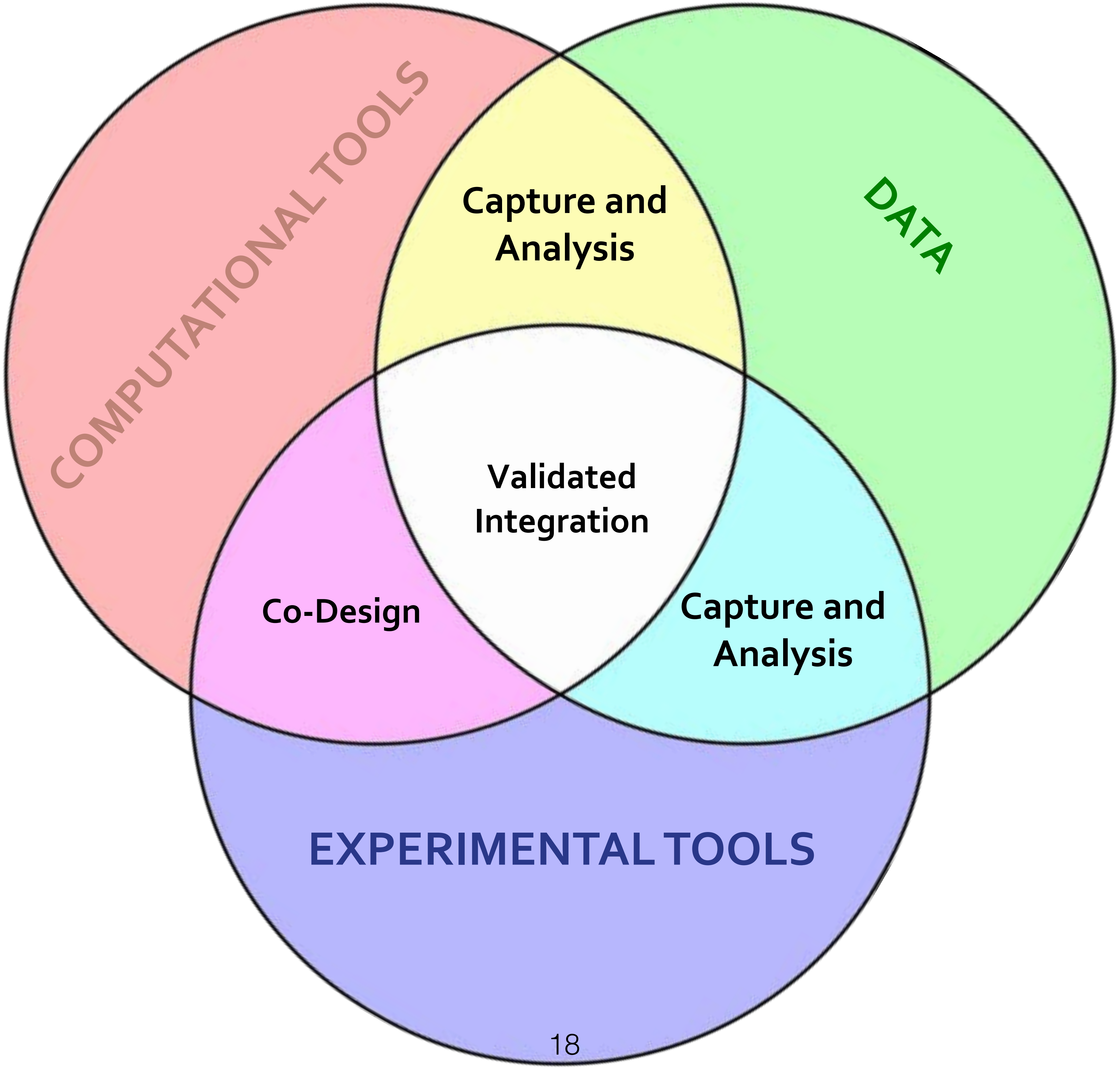
Goal 2: NIST establishes the *means to ensure the quality* of materials data and models

Goal 3: NIST establishes *new methods, metrologies and capabilities* necessary for accelerated materials development.

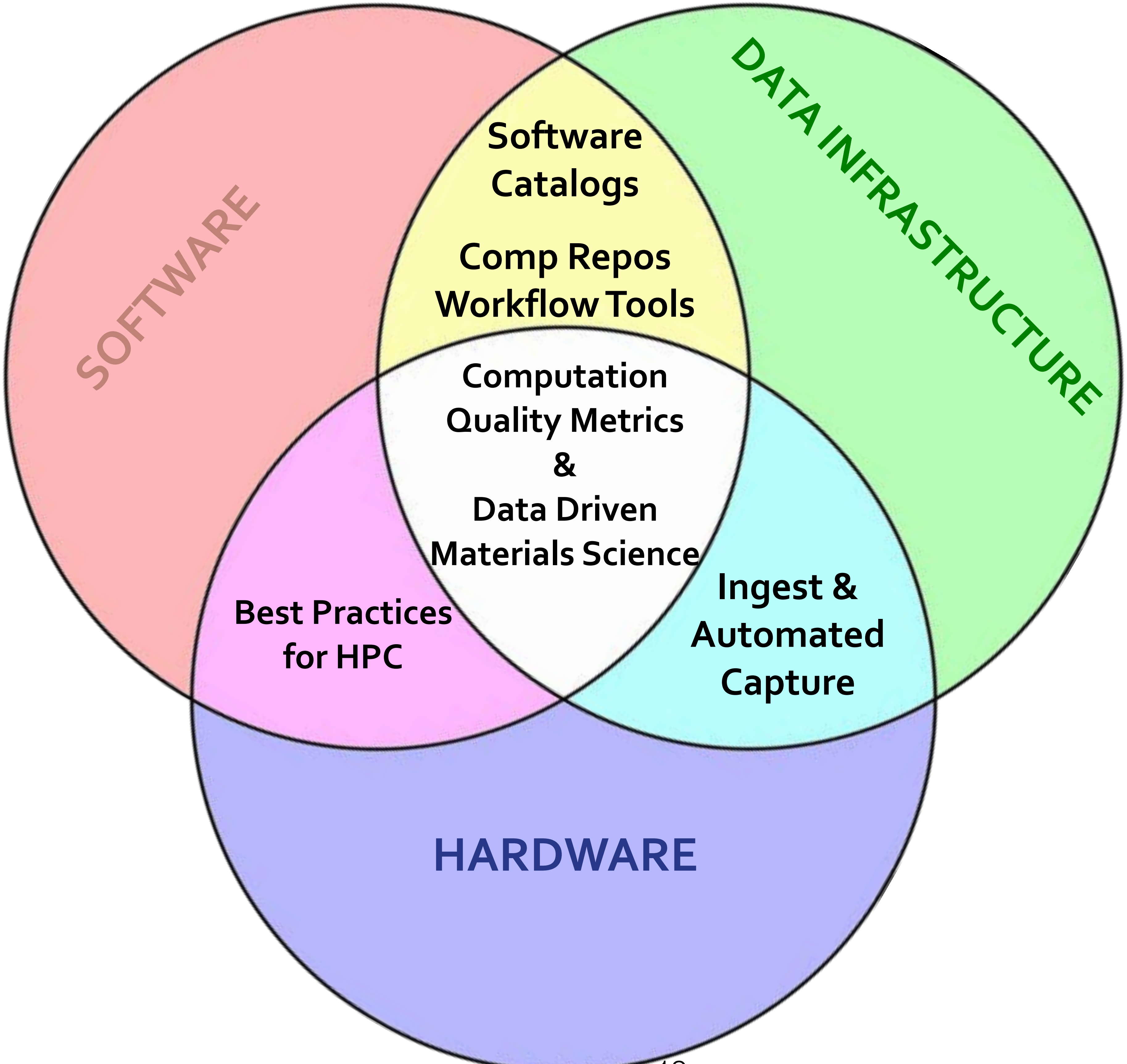
The NIST Portfolio and Wider Questions about Data

MGI.NIST.GOV

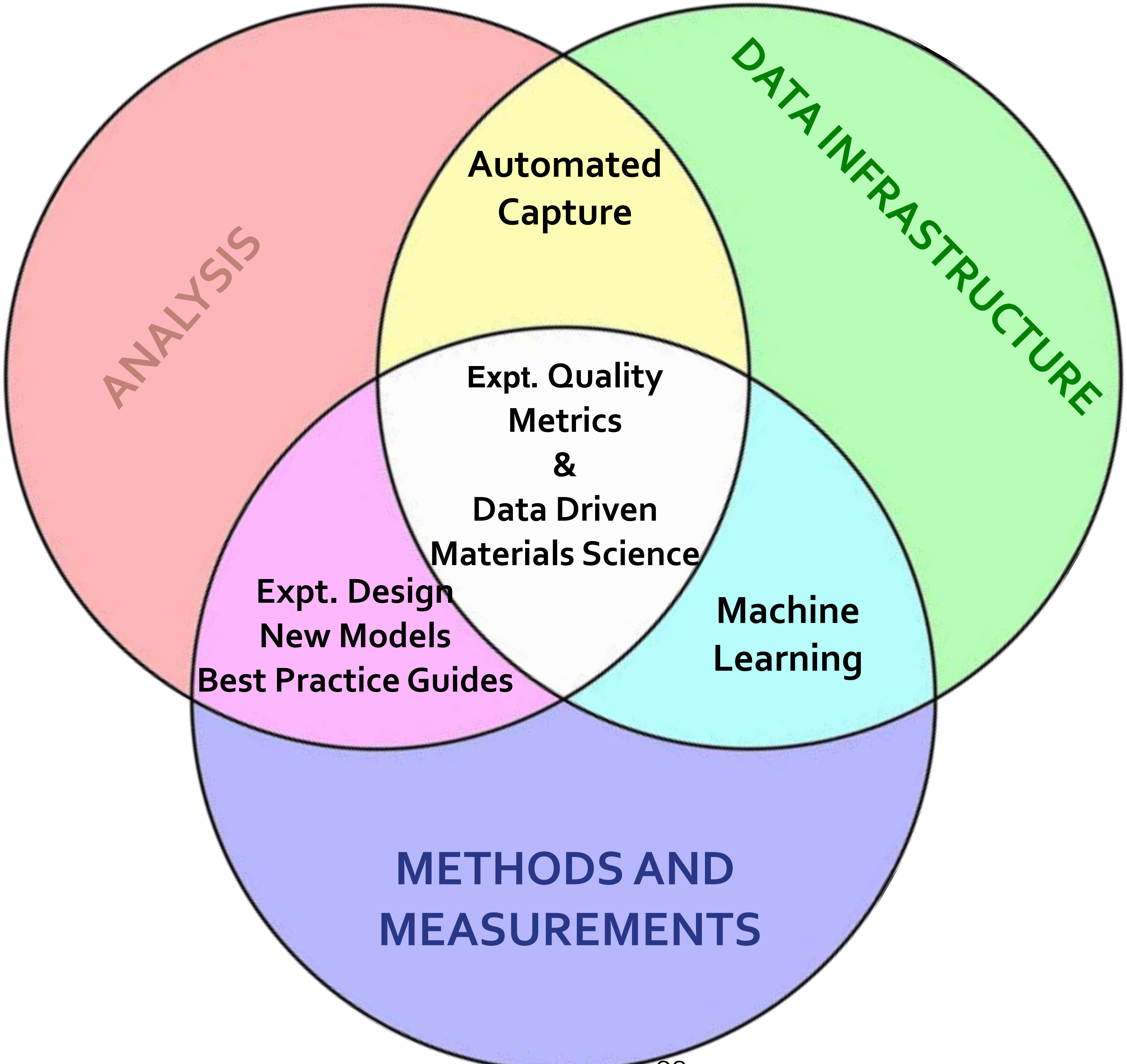
MGI


COMPUTATIONAL TOOLS
DATA
EXPERIMENTAL TOOLS
Capture and Analysis
Validated Integration
Co-Design
Capture and Analysis

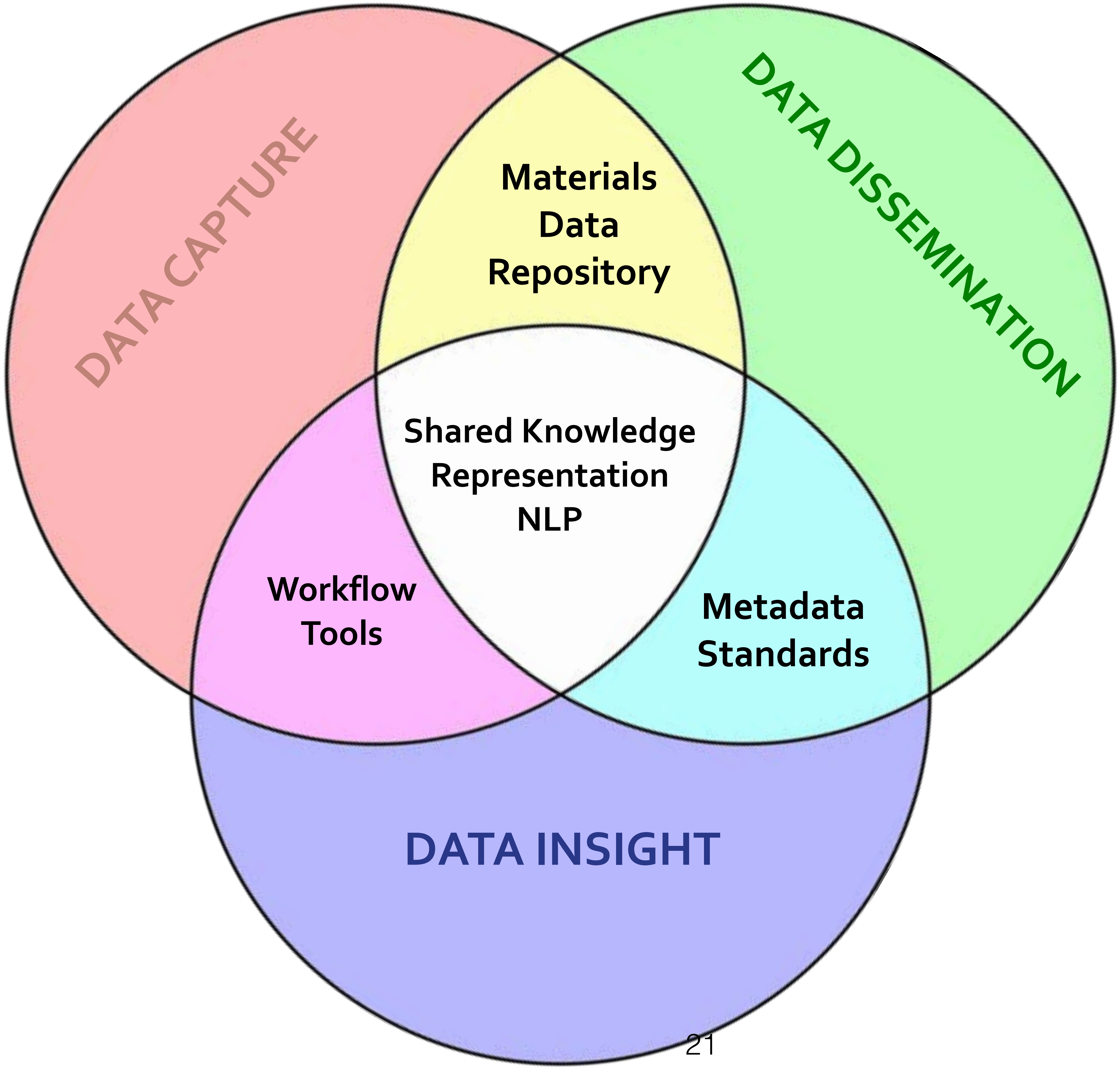
Computational Tools



Experimental Tools



Data


DATA CAPTURE
DATA DISSEMINATION
Materials Data Repository
Shared Knowledge Representation NLP
Workflow Tools
Metadata Standards
DATA INSIGHT

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

NIST
National Institute of Standards and Technology
U.S. Department of Commerce

What’s NIST, the USG and International Community doing about “Data”

- This is really a helicopter view of the broad issues
- You can hopefully not understand much of this part of talk and it shouldn’t matter
- Many issues
  - getting the data “in”
  - getting the data “out”
  - Evaluating the data for quality
  - Using the data for maximum effect
- Who are we working with, who else is a “player”?

Google Materials

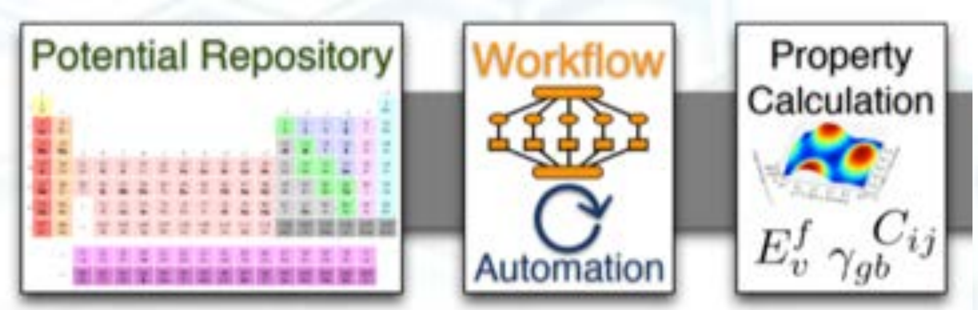
Search

Data Discovery, What do we Need?

1. Some sort of interface/api that the user interacts with to deposit their information such that (2) is enabled. This entails
   a. The establishment of **repositories** to store the data
   b. The reposed data should then be **marked up with sufficient metadata** to inform someone else how the data was created, including attribution or provenance information relevant to citation
   c. Assignment of a **persistent digital identifier** (like the DOI for journals) so the data can be cited and discovered by others
   d. Tools must be developed to
      i. enable the ingest of data from computation or experiment for deposition in a repository
      ii. simplify metadata collection, e.g. by
         1. Automatically assigning some basic metadata
         2. Implementing automatic extraction of metadata to the extent possible
      iii. Assign persistent digital identifiers
2. Some sort of interface/api that the user interacts with to find needed information. This requires (at least)
   a. 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 .
   b. Various types of **policy** enforcement
   c. Tools to evaluate the "**quality**" of the data
      i. Enabling determinations of the data's uncertainty, validity, sensitivity, as well as other metadata qualities
      ii. Enabling assessments of the relevance of the data to the question at hand, such as quick-look plotting or imaging capabilities]
   d. Tools for data manipulation
   e. **Terminologies and ontologies** to enhance search

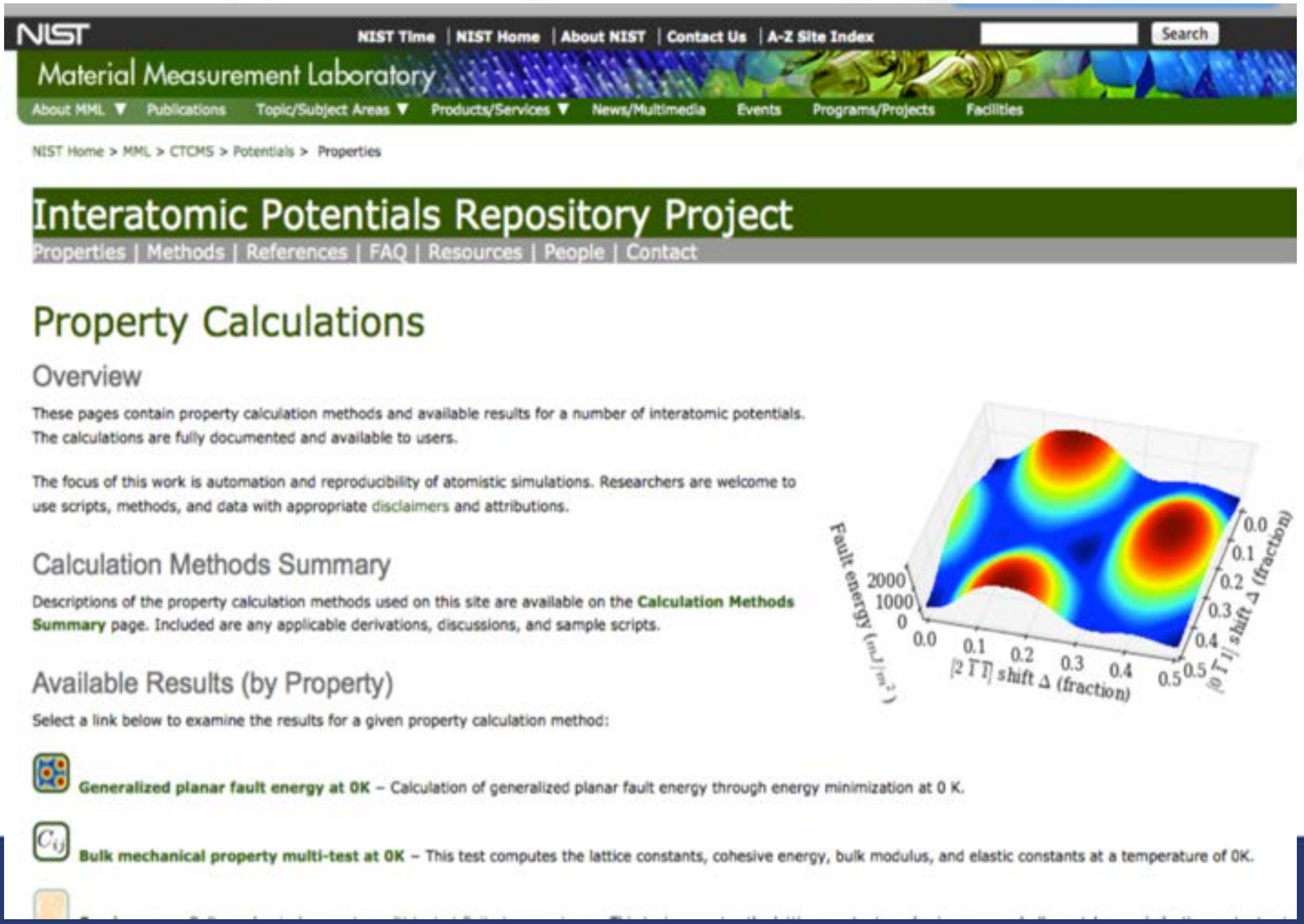
Repositories

Property Calculations on the Interatomic Potential Repository



Zachary Trautt, Materials Measurement Science Division
Chandler Becker, Materials Science and Engineering Division

http://www.ctcms.nist.gov/potentials/



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Material Measurement Laboratory

About MML ▼ Publications Topic/Subject Areas ▼ Products/Services ▼ News/Multimedia Events Programs/Projects Facilities

NIST Home > MML > CTCMS > Potentials > Properties

Interatomic Potentials Repository Project

Properties | Methods | References | FAQ | Resources | People | Contact

Property Calculations

Overview

These pages contain property calculation methods and available results for a number of interatomic potentials. The calculations are fully documented and available to users.

The focus of this work is automation and reproducibility of atomistic simulations. Researchers are welcome to use scripts, methods, and data with appropriate disclaimers and attributions.

Calculation Methods Summary

Descriptions of the property calculation methods used on this site are available on the **Calculation Methods Summary** page. Included are any applicable derivations, discussions, and sample scripts.

Available Results (by Property)

Select a link below to examine the results for a given property calculation method:

Generalized planar fault energy at 0K – Calculation of generalized planar fault energy through energy minimization at 0 K.

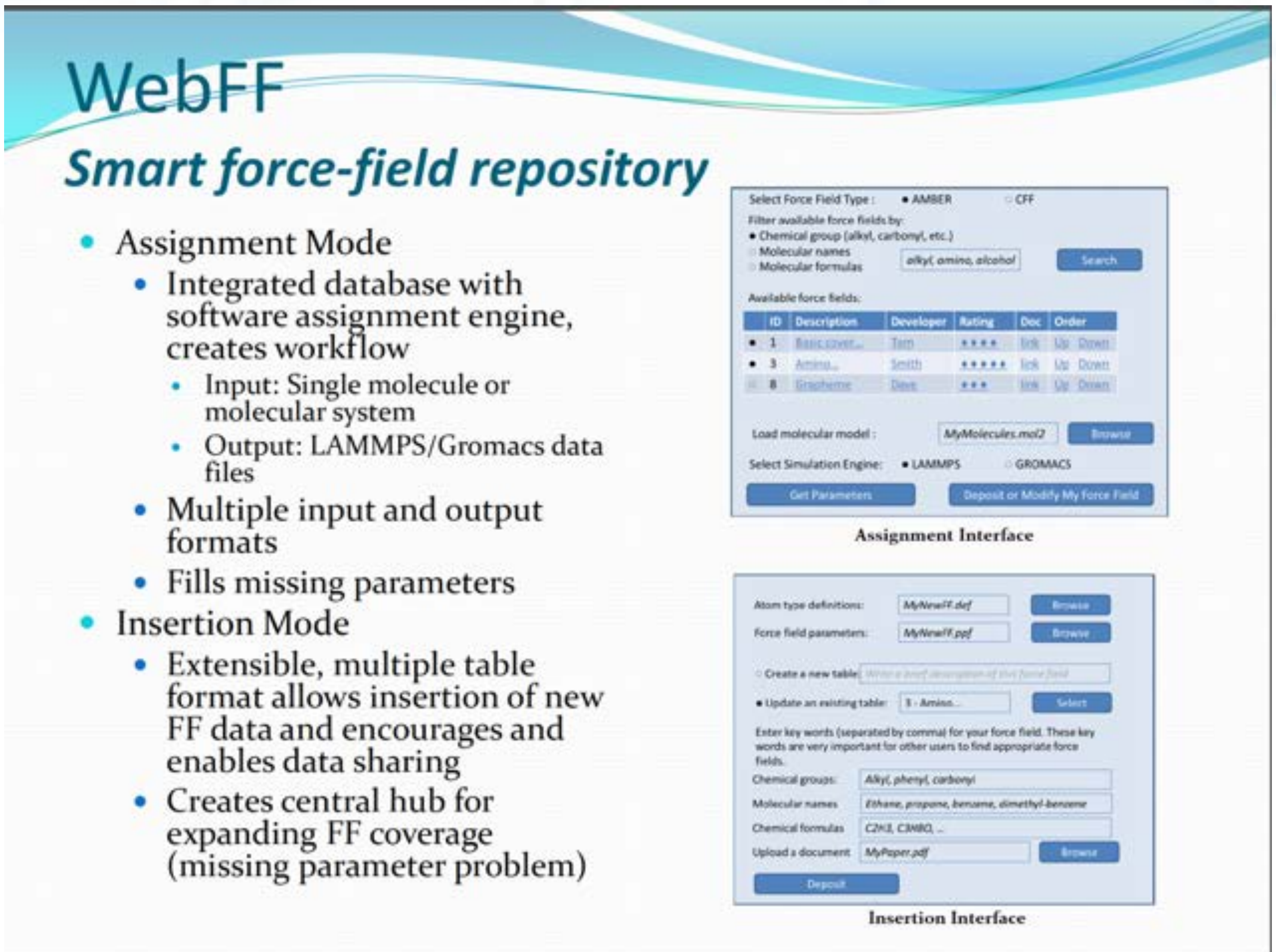
Bulk mechanical property multi-test at 0K – This test computes the lattice constants, cohesive energy, bulk modulus, and elastic constants at a temperature of 0K.

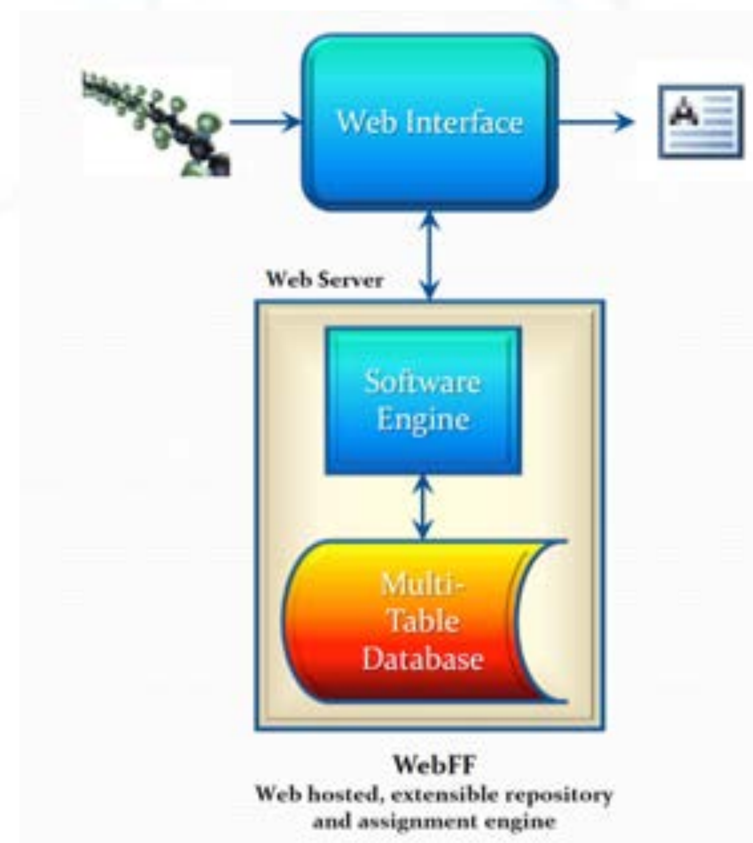
WebFF-A Smart Force-Field Repository of Soft Materials

http://www.nist.gov/mml/msed/polymers/webff.cfm

Frederick R. Phelan Jr. , *Material Science & Engineering Division, Polymers & Complex Fluids Group NIST , Gaithersburg, MD*

Huai Sun , *Aeon Technology Inc. and School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, Shanghai*





https://materialsdata.nist.gov/

Login

NIST

Material Measurement Laboratory

materialsdata.nist.gov

NIST Repositories → Community List

NIST Repositories

The National Institute of Standards and Technology is establishing essential data exchange protocols and mechanisms for widespread adoption to ensure quality materials data and models and to foster data sharing and reuse.

- **CHiMaD Data Collections**
  - **In-Situ Si Composites**
    - In-Situ Si Composites (Si-Cr-Al)
  - **Polymer Nanocomposites**
    - Data for Polymer Nanocomposites
  - **Precipitation Strengthened Alloys**
    - Co-base Alloys
    - Shape Memory Alloys
- **Computational File Repository**
  - Atomistic Simulations
  - CALPHAD Assessments
  - First Principles Phase Stability (FPPS) Files
  - Other Computational Methods
- **Experimental Data Repository**
  - Diffusion Data
  - Molar Volume/Thermal Expansion Data
  - Other Experimental Data
  - Phase Equilibria and Thermodynamic Data
  - **Mechanical Properties**
    - Elasticity Data

Search NIST Repositories

Go

Advanced Search

Browse

All of NIST Repositories

Communities & Collections

Subjects

Titles

Authors

My Account

Login

Customized DSpace repository for materials

➢ Enables sharing of a variety of data types, including text, images, and video

Login

NIST

Material Measurement Laboratory

materialsdata.nist.gov

NIST Repositories → Experimental Data Repository → Diffusion Data → View Item

Data Citation:

Campbell, Carelyn; Zhao, J-C; Henry, M. F.

Examination of Ni-base superalloy diffusion couples containing multiphase regions

(2014-04-02)

http://hdl.handle.net/11256/22 → **Digital Identifier**

Affiliation: National Institute of Standards and Technology, Metallurgy Division, Gaithersburg, MD 20899-8555, USA

General Electric Company, GE Global Research, 1 Research Circle, Niskayuna, NY 12309, USA

Contact Email: carelyn.campbell@nist.gov

Primary Publication Citation:

Materials Science and Engineering A 407 (2005) 135–146

http://dx.doi.org/10.1016/j.msea.2005.07.01

Related Work

Related Publications by Author:

Campbell CE, Boettinger WJ, Kattner UR (2002) Development of a diffusion mobility database for Ni-base superalloys. Acta Mater 50:775-792 DOI: http://dx.doi.org/10.1016/S1359-6454(01)00383-4

Campbell CE, Zhao JC, Henry MF (2004) Comparison of experimental and simulated multicomponent Ni-base superalloy diffusion couples. J Phase Equil Dif 25 (1):6-15. DOI: http://dx.doi.org/10.1361/10549710417966

Abstract:

Four Ni-base superalloy diffusion couples with multiphase regions were studied. The diffusion couples contained single-phase (gamma), two phase(gamma +MC carbide) and three-phase (gamma + gamma prime+MC carbide) regions. Measured average composition profiles were in good agreement with the diffusion simulation predictions. The measured and predicted phase fraction profiles showed similar trends; however, there were some discrepancies in the predicted position of the gamma +gamma prime + MC/ gamma +MC boundary. Phase fraction profiles and optical metallography were used to determine the type and direction of the moving phase region boundaries.

Funding Agency & Award No.:

This work was supported by the Defense Advanced Research Project Agency (DARPA) under the accelerated Insertion of Materials (AIM) Program (Grant number F33615-00-C-5215) with Dr. L. Christodoulou as the project manager and Dr. Rollie Dutton as the project monitor. The authors would like to express their appreciation to N. Saunders for the use of his thermodynamic database for Ni alloys and to Louis A. Peluso, Rebecca Casey, Mitch Hammond and Karen Denike for their experimental support.

Data files

Files in this item

Name: R95-R88-expsimul.txt View/Open
Size: 25.32Kb
Format: Text file
Description:
Experimental and simulate composition profiles for the R88/R95 diffusion couple at 1150 C for 1000 h

Name: r95r88-1000h-labe ... View/Open
Size: 58.76Mb
Format: TIFF image
Description:
Micrograph of R95/R88 diffusion couple after 1000 h at 1150 C

The following license files are associated with this item:

- Creative Commons

Offer licenses with attribution 3.0

This item appears in the following Collection(s)

- Diffusion Data

creative commons

Related items

Showing items related by title, author, creator and subject.

Further Studies on the Nickel-Aluminum System. I. The β-Ni2Al3 Phase Fields

Taylor, A; Doyle, N.J. (1972-01-31)

New lattice parameter and density results have been obtained for alloys in the ß-NiA1 and 6-Ni2A13 phase fields of the nickel-aluminum system. The lattice parameter of the ß-NiAl phase (CsCl-type) falls linearly from ...

Elemental vacancy diffusion for fcc and hcp structures

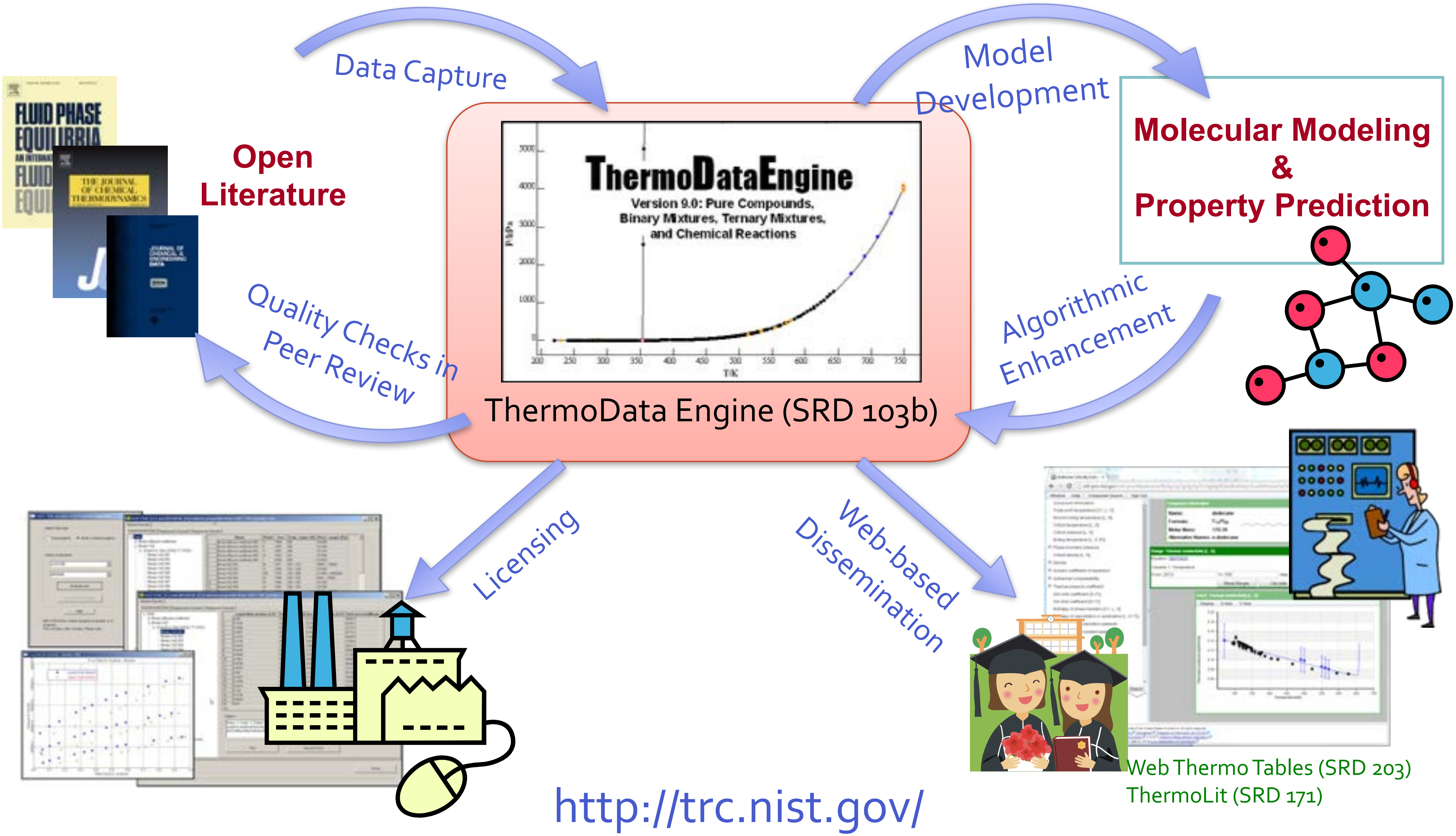
Angsten, Thomas; Mayeshiba, Tam; Wu, Henry; Morgan, Dane (2014-08-08)

This work demonstrates how databases of diffusion-related properties can be developed from high-throughput ab initio calculations. The formation and migration energies for vacancies of all adequately stable pure elements ...

Metadata Curation

Markup

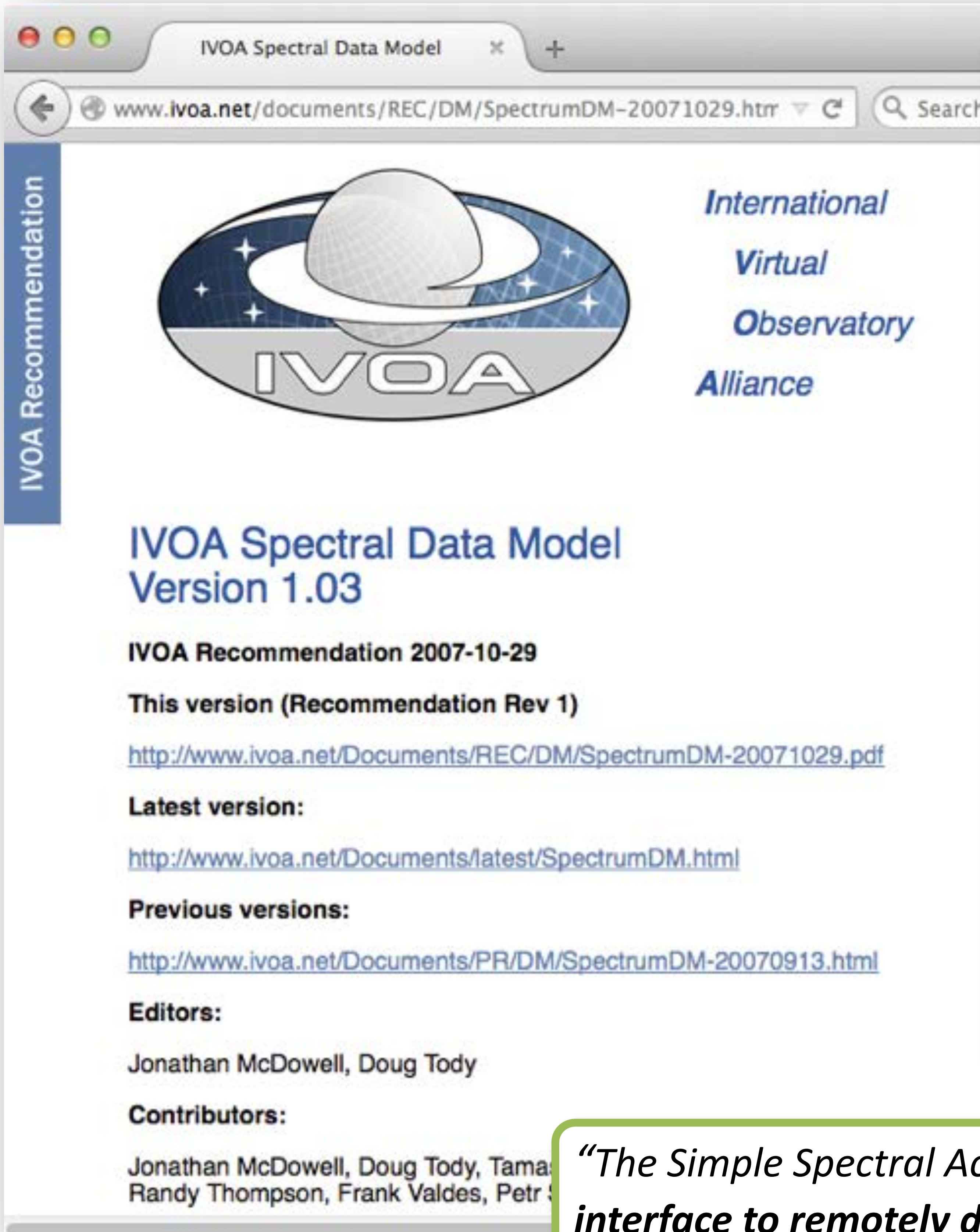
THERMODYNAMICS RESEARCH CENTER



- Expanding to metallic systems
- Initial focus on phase equilibria data and thermochemical property data .

Vision of Materials Data Curation System

A Successful Example



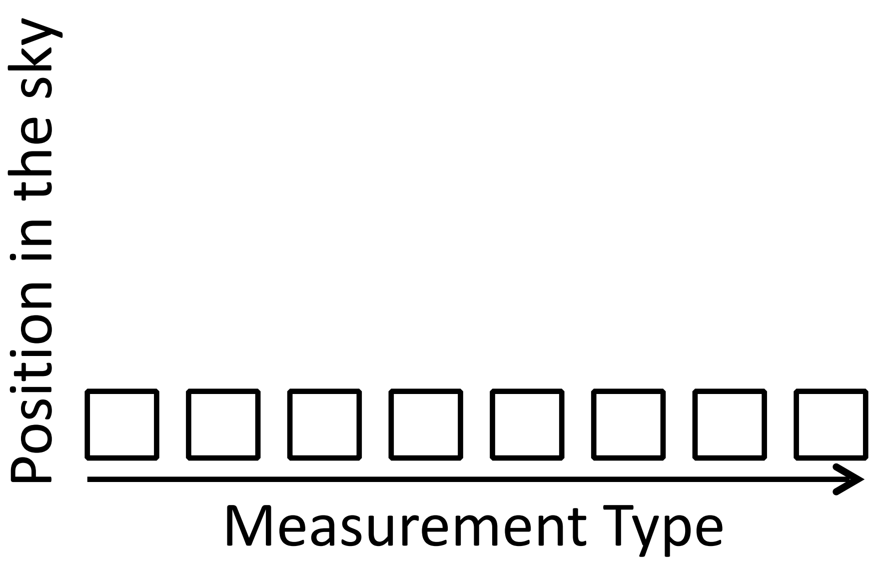
*"We present a **data model describing the structure of** spectrophotometric **datasets** with spectral and temporal coordinates and **associated metadata**. This data model may be used to represent spectra, time series data, segments of SED (Spectral Energy Distributions) and other spectral or temporal associations."*

*"In this document we present a proposed abstraction for spectral data and serializations in VOTABLE, FITS, and XML, for use as a **standard method of spectral data interchange**."*

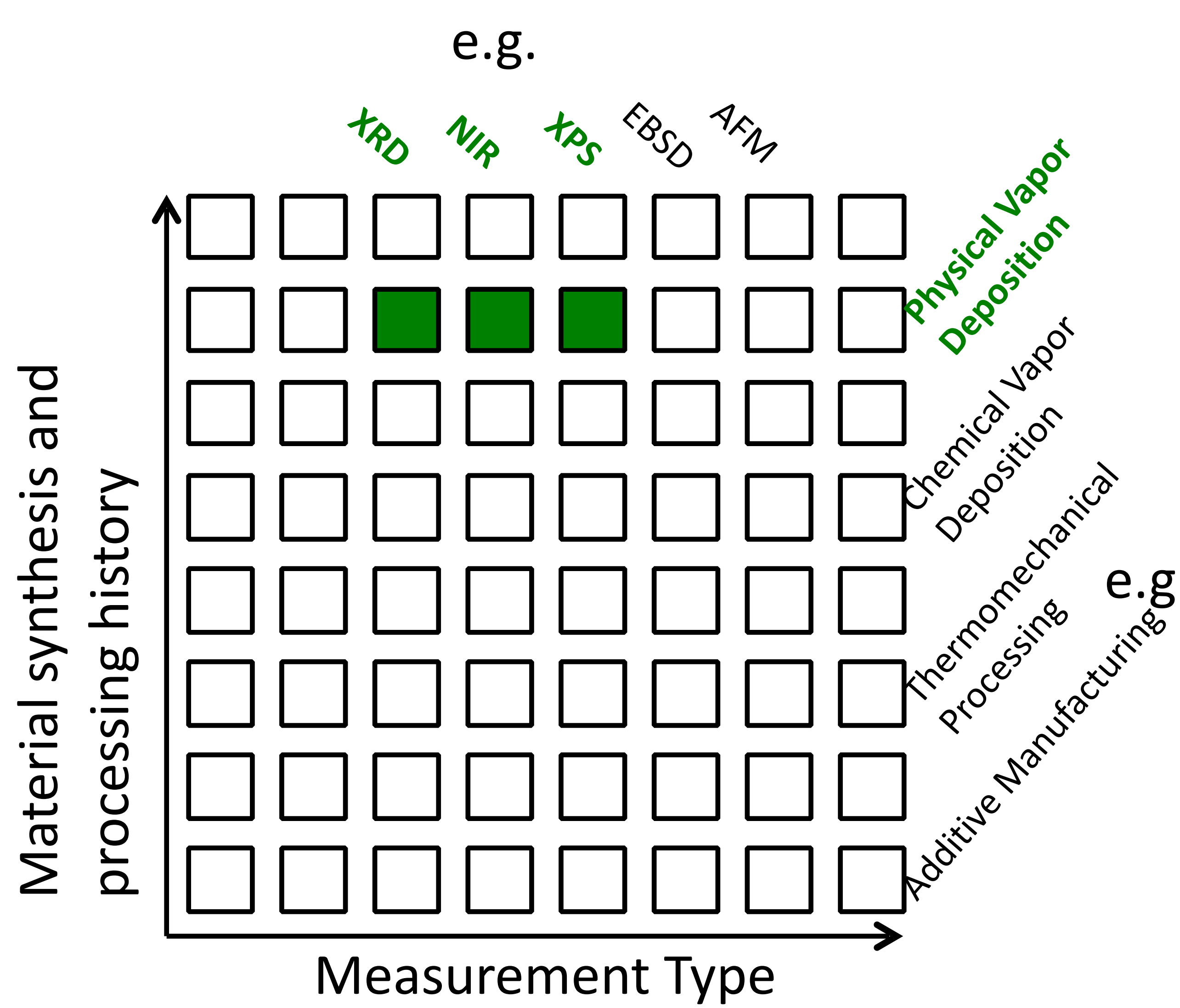
*"This is a Proposed Recommendation, developed with the intention to **support the Simple Spectral Access Protocol**."*

*"The Simple Spectral Access (SSA) Protocol (SSAP) defines a uniform **interface to remotely discover and access** one-dimensional spectra."*

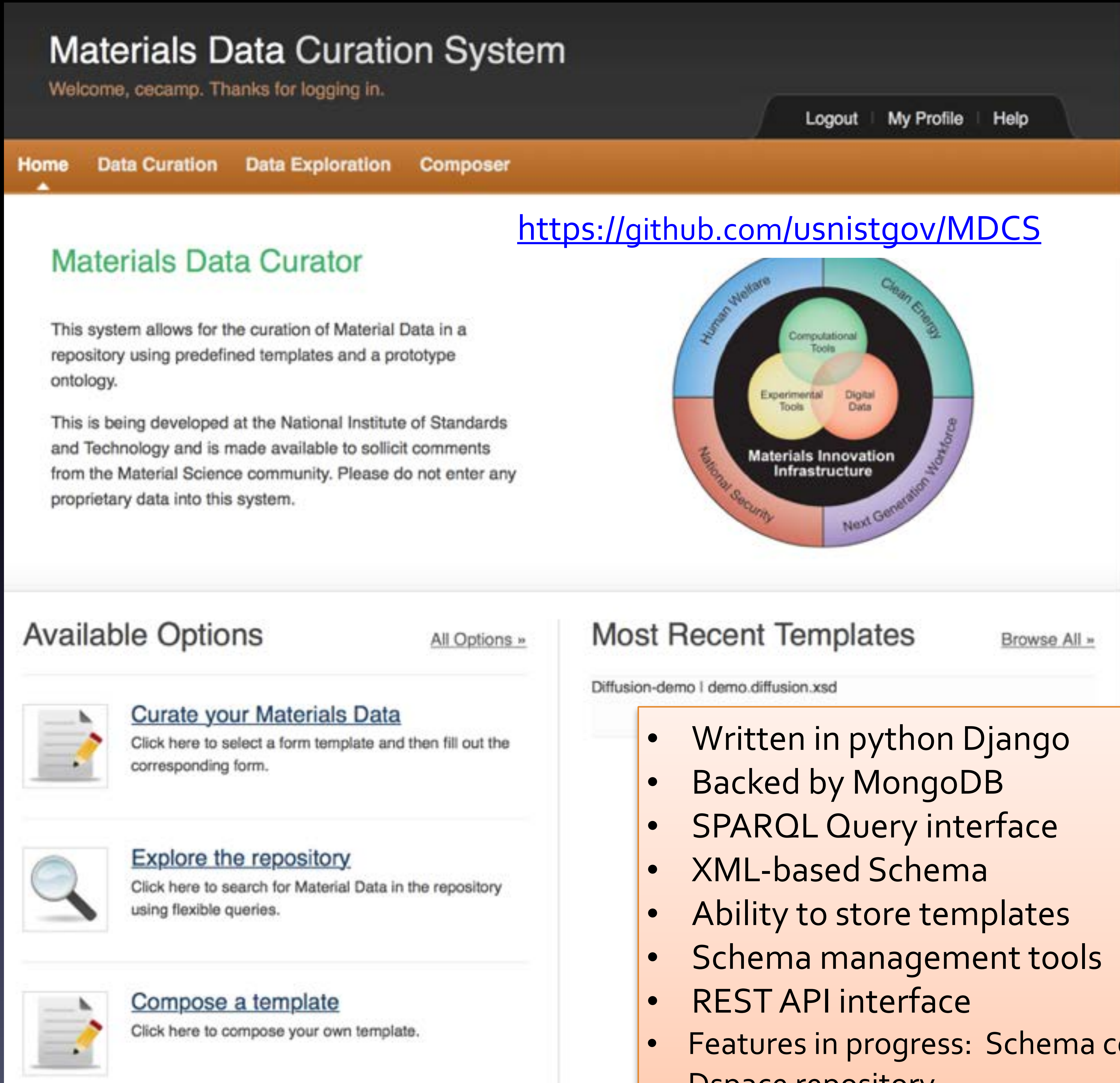
Astronomy vs. Material Measurement



Singular data models



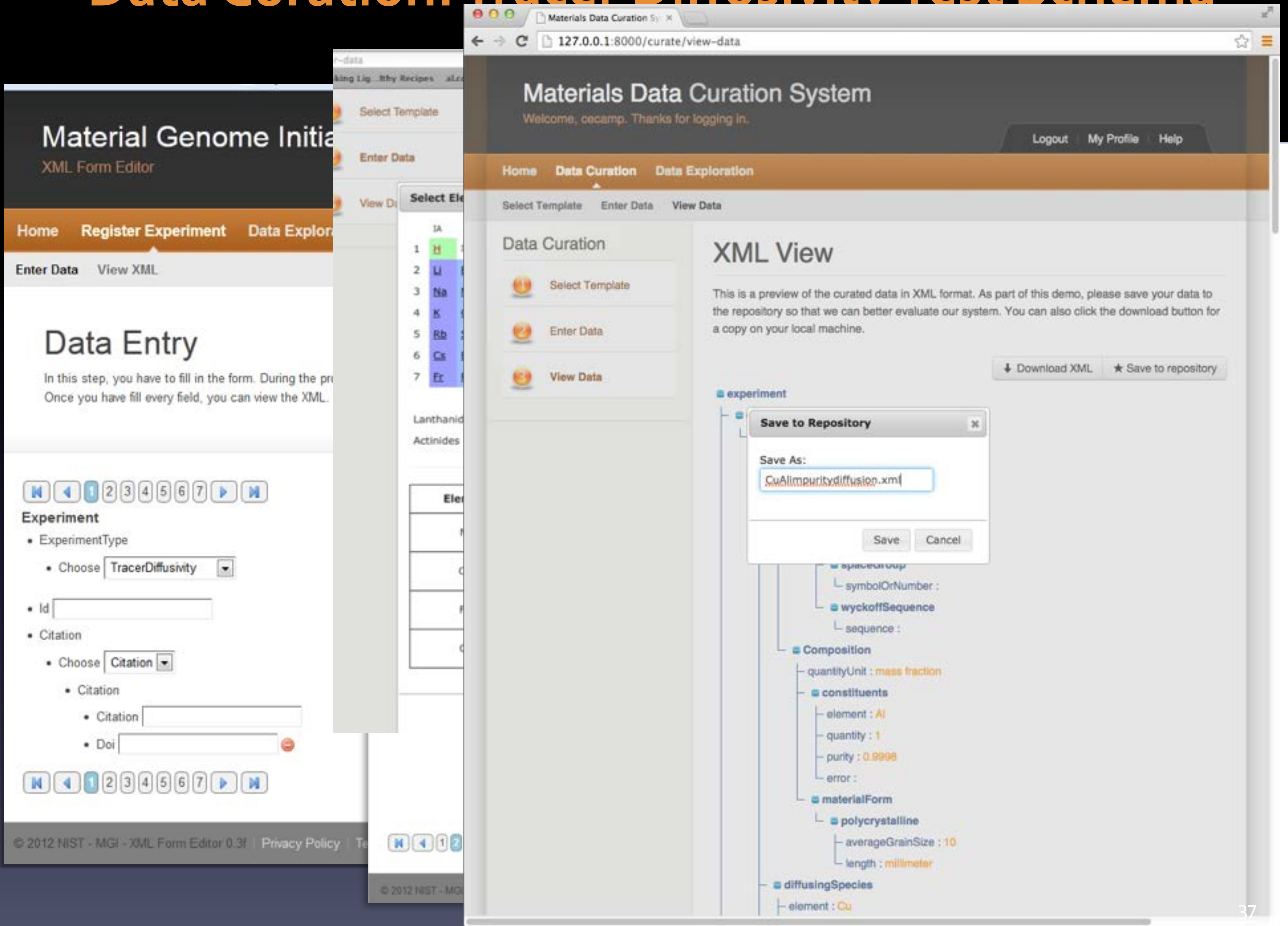
Modular data models



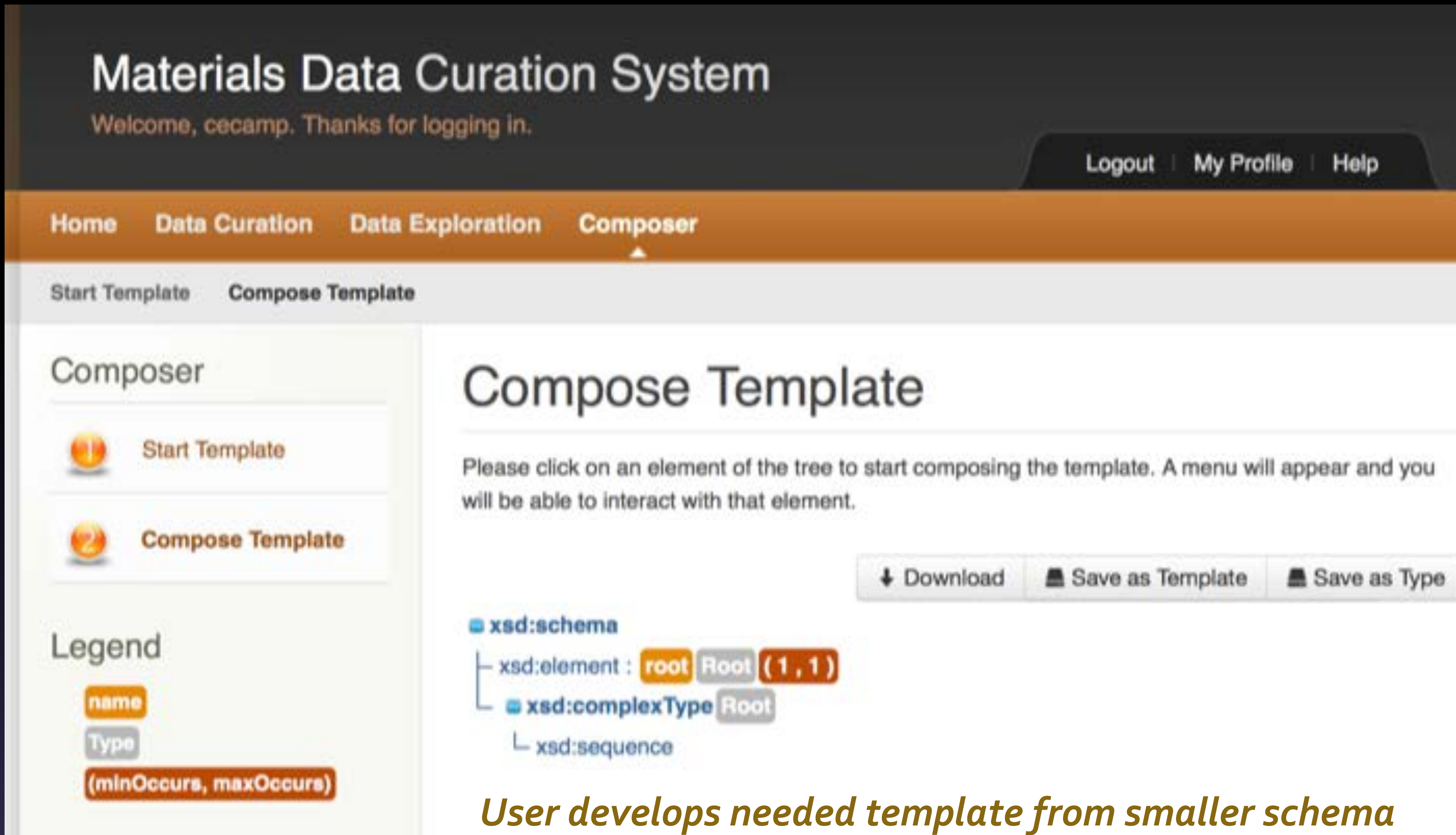
https://github.com/usnistgov/MDCS

- Written in python Django
- Backed by MongoDB
- SPARQL Query interface
- XML-based Schema
- Ability to store templates
- Schema management tools
- REST API interface
- Features in progress: Schema composer and Links to Dspace repository

Data Curation: Tracer Diffusivity Test Schema



Development of Composer



User develops needed template from smaller schema

Material
- Metals
  - Al Alloys
  - Fe Alloys
  - Ni Alloys
  - ....
- Polymers

Processing
- Heat Treatment
- Casting
- Thermomechanical processing
- Sintering
- Rapid Cooling
- …

Sample Preparation
- Polishing
- Etching
- Electro-polishing
- .....

Measurement Method
- EPMA/EDS
- EMSD
- DSC/DTA
- Dilatometer

Application Programming Interface *in a nutshell*

WWW interface to the Curator:

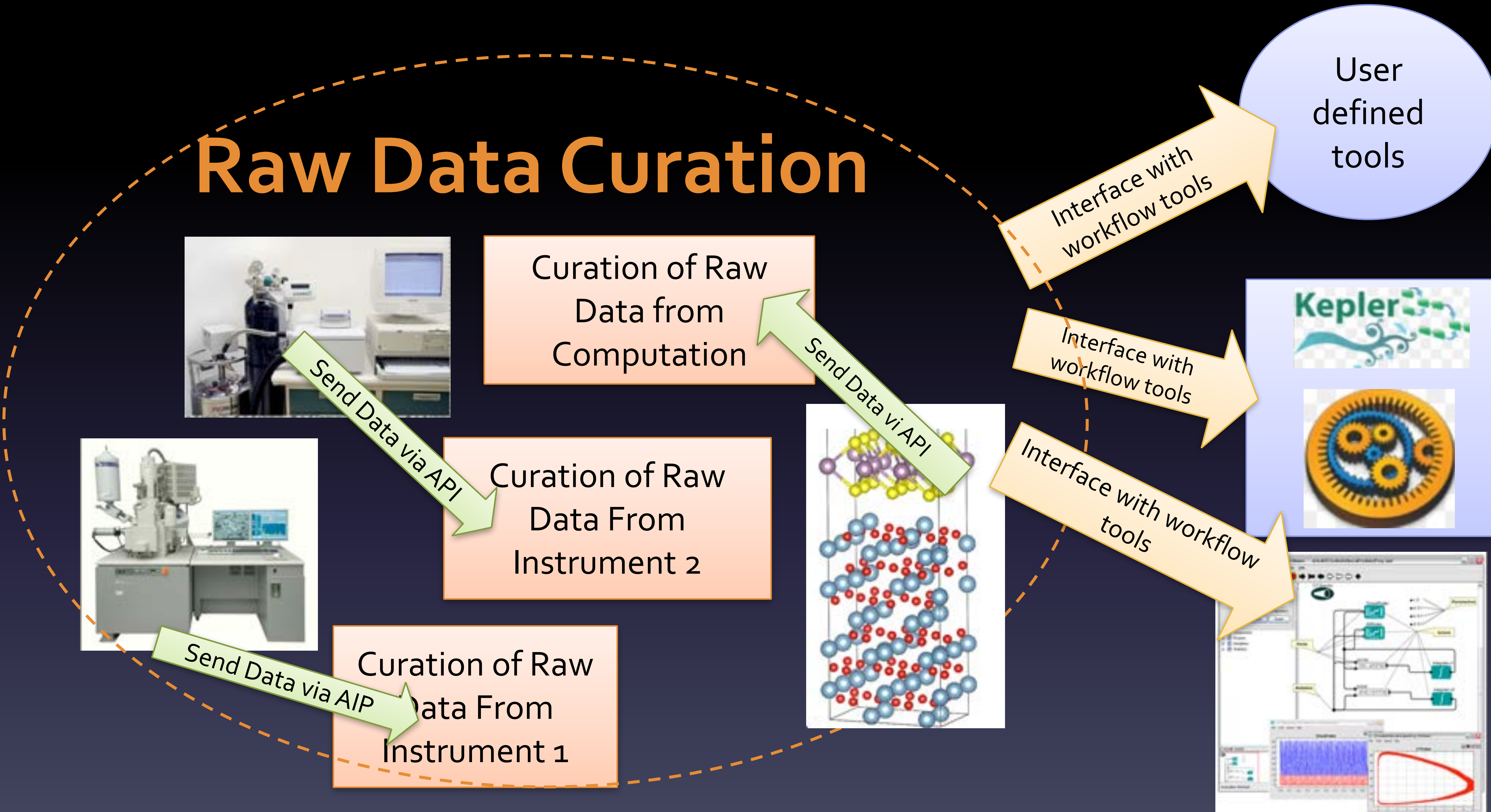
API interface to the Curator:

Hand data entry

Automated data entry

Materials Data Curator Use Schematic

First Step Curate Raw Data



Registries

National Institute of Standards and Technology

NIST National Institute of Standards and Technology U.S. Department of Commerce

The case for a Materials Resource Registry

Register. Discover. Access.

Research Data Alliance

National Institute of Standards and Technology (NIST)

National Data Service (NDS)

Center for Hierarchical Materials Design (CHiMaD)

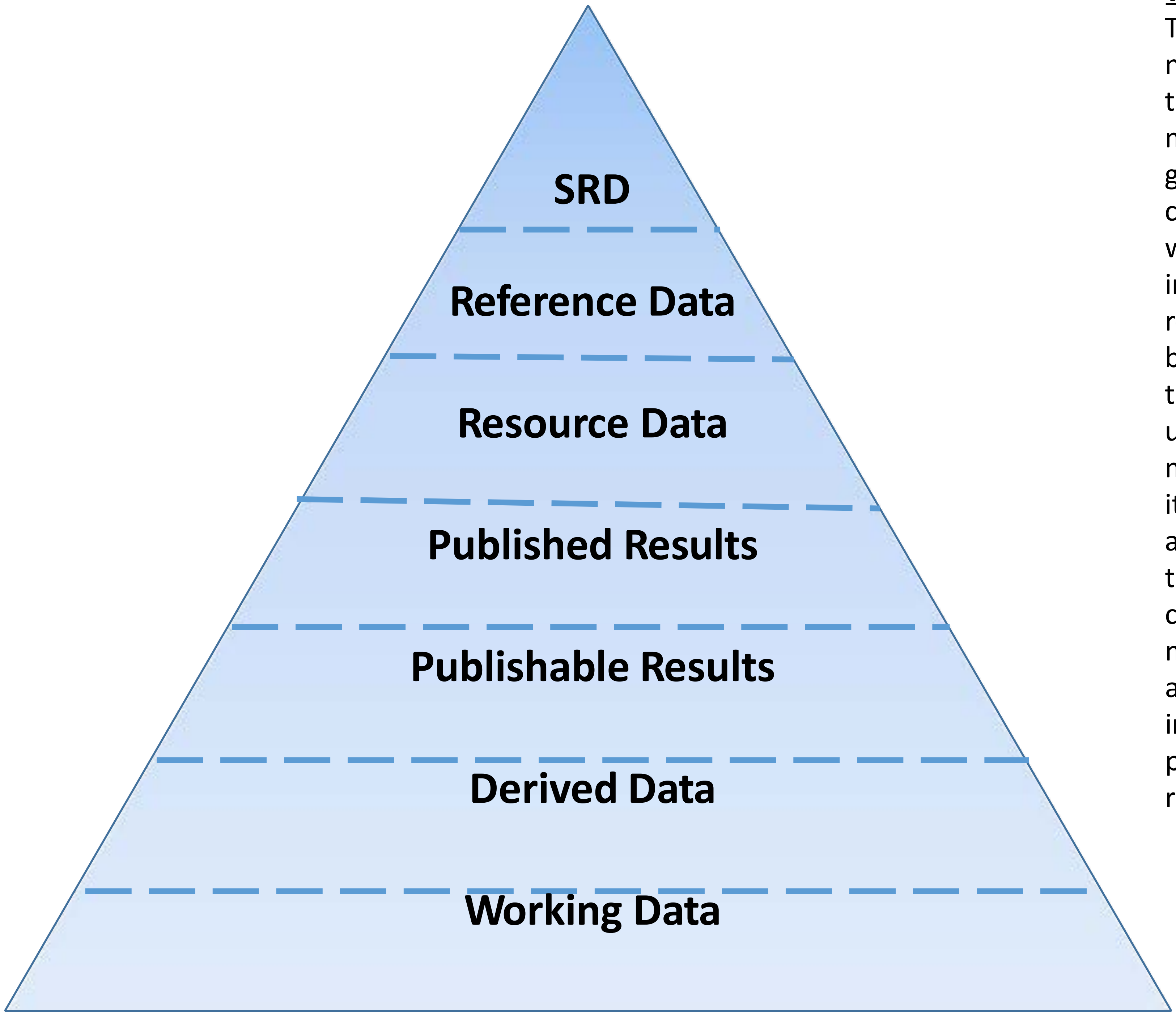
Research Data Alliance (RDA)

Collaborators

Data Policy

A NIST Approach (in progress)

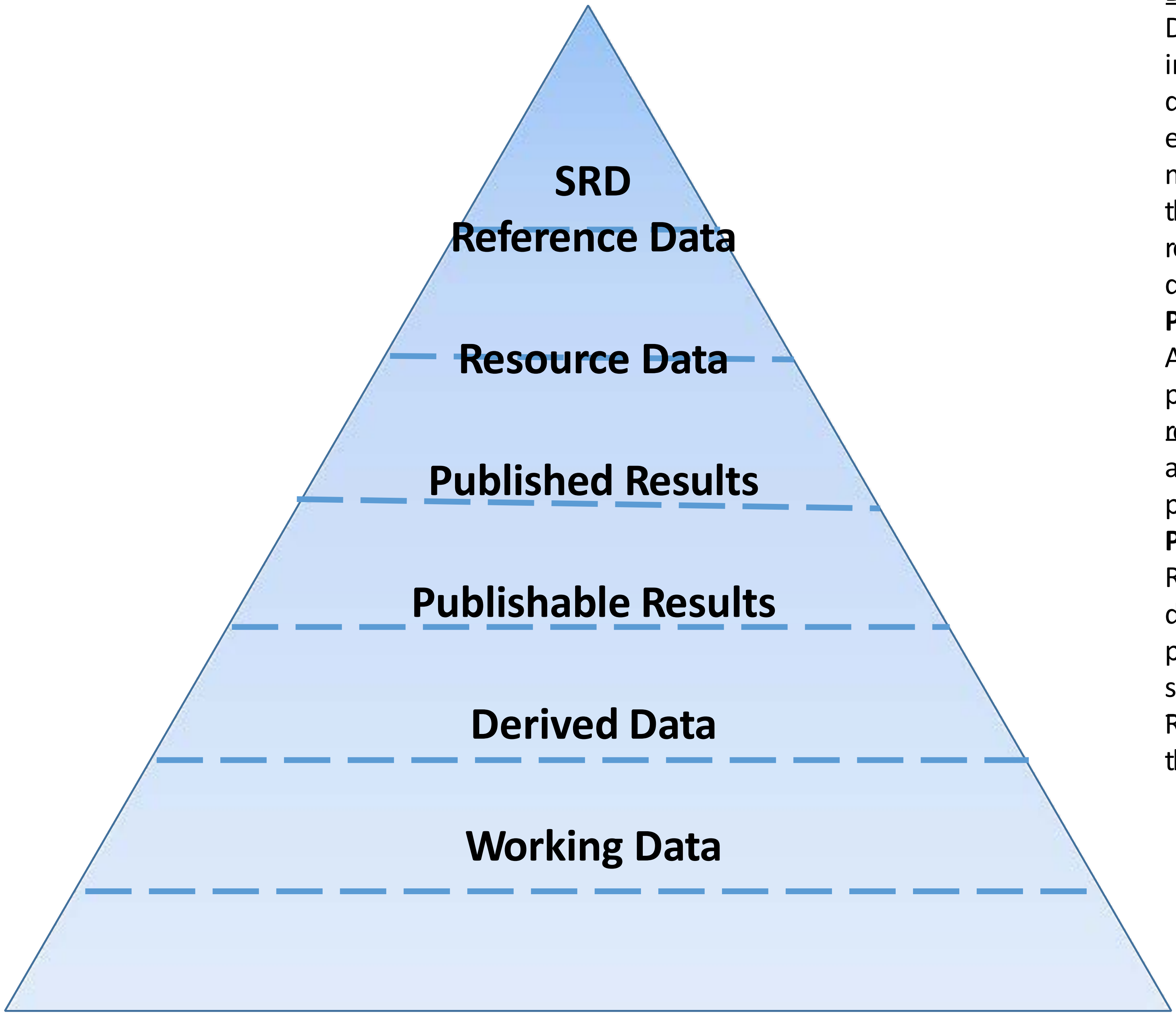
Data Taxonomy: STRAWMAN-DRAFT



Working Data

The digital equivalent of entering data in a laboratory notebook. Working data may be raw observational data that is acquired directly from an instrument or a measurement system, or digital values acquired or generated during experiments or simulations. In some cases the researcher responsible for generating the working data may determine that this data has immediate value and is worth preserving, or the researcher expects the data will have value after it has been manipulated or further evaluated, and the data has the potential to develop into a publication or will be used to draw conclusions. In other cases working data may be recognized as not appropriate for broader use in its present form. It may have value to the data producers and their collaborators, but it should be recognized that the data could be easily misinterpreted by people not closely involved in its production because some metadata and important facts about its status or acquisition are not readily available beyond the immediate research team (i.e. adequate metadata for re-purposing is not attached to the data itself, expending resources to codify needed metadata is not justified, etc

Data Taxonomy



Derived Data

Derived data are those that underpin the conclusions provided in a publication or report. Derived data come from working data that have been manipulated, analyzed, processed, or evaluated in some way. The data must have passed some minimal (perhaps ad hoc) evaluation and be considered by the responsible researcher (typically the data producer) to be ready for the next steps in the workflow or project/product development effort.

Publishable Results

All final or summary results that comply with relevant NIST policies (e.g., SI units, uncertainty statements), that have been reviewed internally and approved by an appropriate NIST authority, and that could be published either in a scientific publication or as a standalone data product.

Published Results

Results that are publishable and that are contained in a document that has been reviewed and approved for publication by the necessary NIST organizational authorities, submitted to its intended publisher, and made public. We see ~~Reports of Analysis~~ as fitting in this category but no longer call them out because they seem unique to MML.

Data Taxonomy: STRAWMAN-DRAFT

- Preservation Levels
  1. No additional requirements
  2. Individual user responsibility
  3. Data backed up using a tested/automated process

- Discoverability Levels
  1. No additional requirements
  2. Persistent Identifier (PID) assigned
  3. Entered in NIST Enterprise Data Inventory[1]
  4. Inventory record flagged for public access

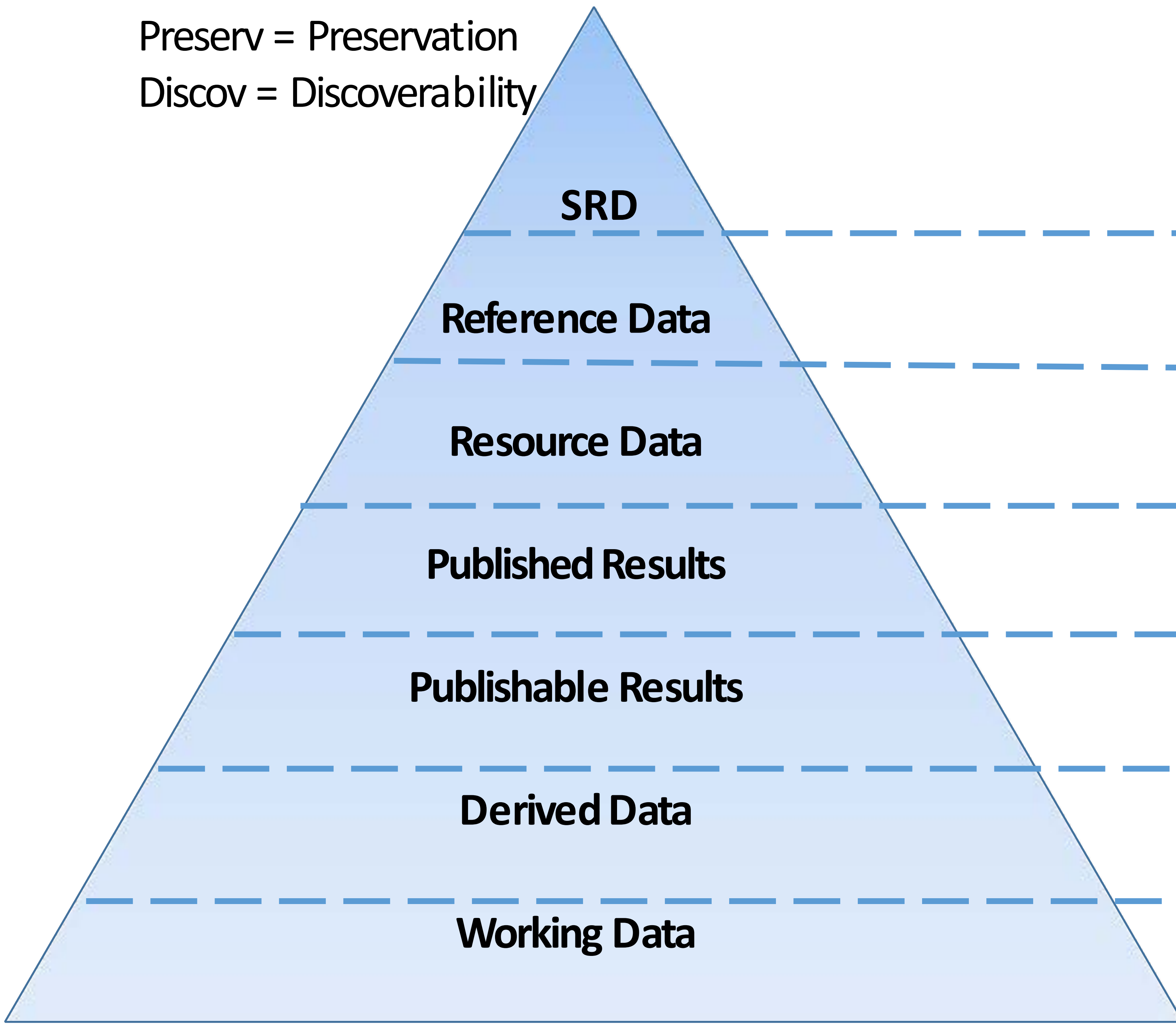
[1]PID assigned + NIST minimum metadata present

Data policy under discussion

mapping levels onto categories

STRAW MAN-DRAFT

Preserv = Preservation
Discov = Discoverability



Preserv	Discov
3	4
3	4
3	4
3	4
2	3
1	1
1	1

Collaborations
Discussions
Convening

RESEARCH DATA ALLIANCE

Research Data Sharing without barriers

Research Data Alliance Interest Group

RDA/CODATA Materials Data, Infrastructure & Interoperability IG

James A Warren and Laura Bartolo, Co-Chairs

Materials Resource Registry, Working Group, *Robert Hanisch, Chair*

Exploration of Opportunities

EMMC

- The aim of the council (for the moment) is to do preparatory networking to establish activities necessary in the materials modelling field.
- The Council could build on existing activities happening in Europe and make use of the network to complement these activities.

National Data Service

HOME ABOUT EVENTS WIKI GET INVOLVED

THE NATIONAL DATA SERVICE

The National Data Service is an emerging vision of how scientists and researchers across all disciplines can find, reuse, and publish data. It is an international federation of data providers, data aggregators, community-specific federations, publishers, and cyberinfrastructure providers. It builds on the data archiving and sharing efforts under way within specific communities and links them together with a common set of tools.

VISION

It is widely believed that ubiquitous digital information will transform the very nature of research and education. The reasons for this excitement are clear: In essentially every field of science, simulations, experiments, instruments, observations, sensors, and/or surveys are generating exponentially growing data volumes. Information from different sources and fields can be combined to permit new modes of discovery. Data, including critical metadata and associated software models, can capture the precise scientific content of the processes that generated them, permitting analysis, reuse, and reproducibility. By digitizing communication among scientists and citizens, discoverable and shareable data can enable collaboration and support repurposing for new discoveries and cross-disciplinary research enabled by data sharing across communities. Open, shareable data also promise to transform education, society, and economic development.

However, while some communities are making progress in developing discipline-specific data services, the U.S. and international scientific communities lack a unified framework and supporting services for storing, sharing, and publishing data; for locating data; or for verifying data. More specifically, we are lacking standard means of

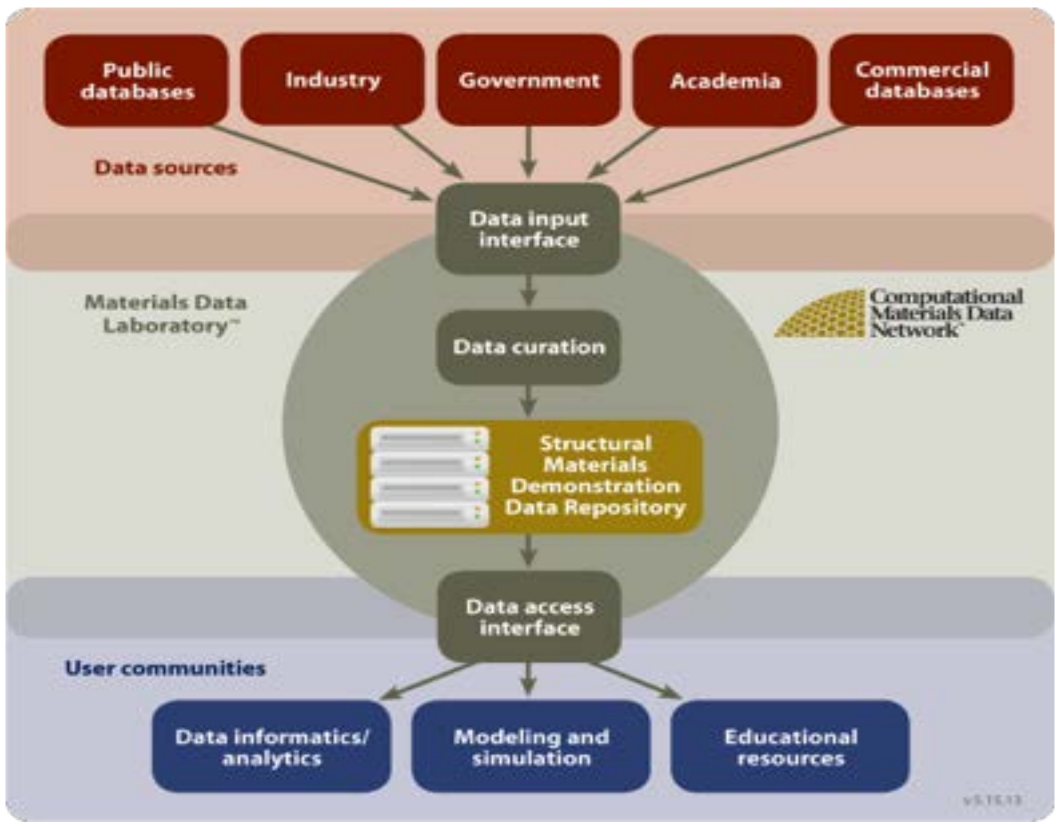
NEWS

The launch of Materials Data Facility in support of Materials Genome Initiative

06.19.14

The National Data Service Consortium to launch a materials data facility for the advancement of materials science research through open data access and sharing. **Read more**

Structural Data Demonstration Project: Al6061



March 2014: Phase 1 release.
June 2014: Phase 2 release.
Dec 2014: Project Completion

Goal: Establish well-pedigreed and curated demonstration datasets for non-proprietary metallic structural materials data over all length scales.

NIST's role

- Provide data schemas and meta-data formats for diffusion and phase equilibria data.
- Provide sample diffusion and phase equilibria data for the Al-Mg-Si system.
- Use expanded TRC Guided Data Capture program with available binary and ternary phase equilibria literature
- Expand use and implementation of DSpace Repository
- Link with developing ontology and semantic web tools

NIST Center of Excellence for Advanced Materials

CHiMaD | Center for Hierarchical Materials Design

NIMS

CHIMaD Center for Hierarchical Materials Design

NIST

NSF

First US-Japan MGI Workshop, June 2015

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