Working Group 6: CALPHAD Proto Data

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

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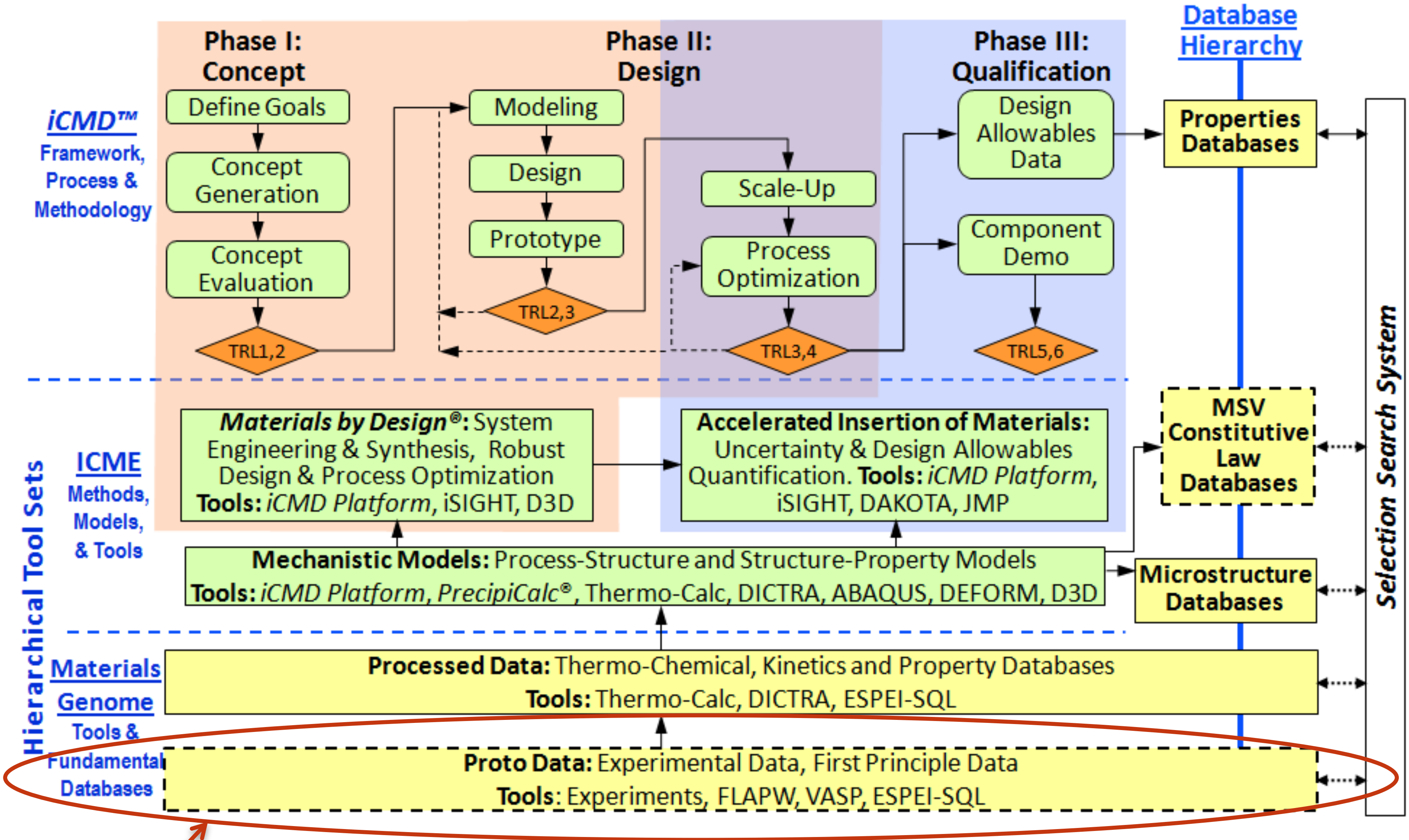
Significance of WG's Focus

- Generation, curation and dissemination of CALPHAD files (e.g. TDB, POP, etc) and CALPHAD proto data.

- CALPHAD Proto Data: Phase-base property data (temperature, composition, and pressure dependent)
  - Data are diverse
  - Data semi-structured

Data and files are essential for the development of multicomponent databases that serve as a building block for materials design.

Basis of data tools and schemas develop are material class independent.



Focus (phase-based property data needed to build
Composition, temperature, pressure dependent CALPHAD-base databases

G. B. Olson, 2013

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Summary of WG's Goals

- Improve the dissemination/discovery of CALPHAD files, including functional descriptions, evaluated data, and macros/scripts (eg. TDB, POP, TCM, etc)

- Improve the curation and dissemination of CALPHAD proto data
  - Developing curation tools and schemas
  - Establish best practices (e.g. ThermoML 5.0 for the curation of thermodynamic data)

Goal: Implement Co data for Spring Design Project

- Distribution existing work Feb 2016
- Assemble available experimental data in the MDCS as possible (thermodynamics, diffusion, DFT)
  - Refinement of data schemas
  - Add Re to existing Co-base descriptions (Co-Al-W-Ni-Ti-Ta-V) to Questek database (Co-C-Al-Cr-Fe-Mn-Ni-Ti-V-W)
  - Deadline: End of March
- Distribute available TDB/POP files (Dspace – CHiMaD only community)
  - During the design course
- Demonstrate search strategy for component selection using Granta software
  - Short term Goal: Shared data schemas and implement common search strategies in Granta and MDCS
  - Long term Goal: Indexing a federated system

Technical Requirements/Needs

- Dissemination of CALPHAD files
  - Ease of use (input and discovery)
  - Flexible inputs
  - Ability to link to additional resources (e.g files)

- Curation of CALPHAD proto data requires a system able to
  - Handle diverse data sets: computational and experimental, from single data points to complex 3D atom probe data
    - Need modular data schemas
  - Transform data into new formats
  - Combine data from multiple sources
  - Find data and reuse it
  - Associate metadata with data values
  - Automated data curation and search (REST API)

Solutions/Actions

- Dissemination of CALPHAD files
  - Where
    - NIST Dspace Repository:CALPHAD Assessments community
    - Materials Data Facility
    - Journals (JPED, CALPHAD –subscribers only)
  - How: Need to encourage publishers to require files and link data resources
- Curation of CALPHAD Proto data
  - Evaluate available and developing tools
  - Evaluate data curation schemas
  - Engage the community in using developed tools and developing needed data schemas

Data Curation/Archival Tools

- MDCS/ThermoML (https://github.com/usnistgov/MDCS)
- Granta MI (http://www.grantadesign.com/products/mi/) commercial
- Citrine (http://citrination.com/)
  - Focused collection
- Materials Commons
  - (http://www.prisms-center.org/#/mcommons/overview)

ESPEI-V2 – pre-CALPHAD data assessment tool (Penn State)

Evaluation of Materials Data Curation Tools

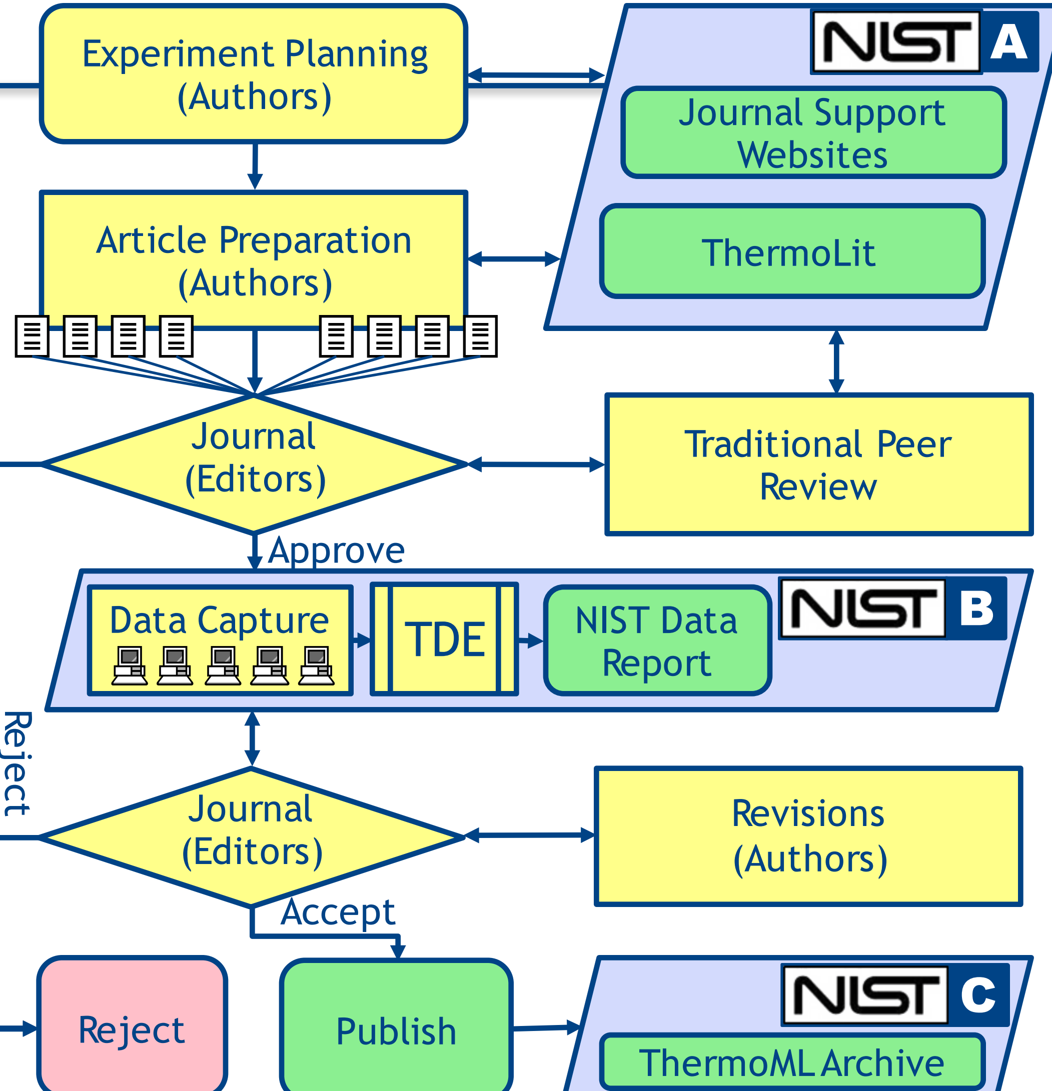
	MDCS	Materials Commons	Granta MI	Citrine
Data import formats	Anything	Anything	Excel-based, cvs, tabular	Excel, cvs, tabular
Image/Large Data capability	Yes	Yes	Yes (limited)	??
Data stored as	XML	JSON	Modified MatML	JSON
REST API	yes	yes		Yes?
Data Storage	MongoDB	ReThinkDB	Relational DB	??
Type of Code	Open	Open	Commercial	Partially??
Data output	Anything (future)	Anything (future)	Excel, cvs, mod-MatML, code specific	???

Solutions/Actions

- Evaluation of ThermoML V5 for the curation of thermodynamic data (applications to metals and alloys) test in terms of Co-base superalloys
  - Test draft schema with data from participants (computational and experimental)
  - Evaluate the how to extend or re-use parts of ThermoML for other phase-based properties (i.e. diffusion)

Journal Cooperation

- According to statistics gathered at TRC, 1 in 3 articles has a fundamental issue in its reported data
- What is NIST doing to help repeatability in science?
- Since 2003, TRC has collaborated with 5 journals to stem the flow of erroneous data
  - Present workflow in place since 2013
- We work with IUPAC and:
  - *Journal of Chemical and Engineering Data*
  - *Fluid Phase Equilibria*
  - *The Journal of Chemical Thermodynamics*
  - *International Journal of Thermophysics*
  - *Thermochimica Acta*
- Our experts review 1000 articles per year and fix 500 issues per year



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Collaborations/Synergies

- Inputs need from other working groups
  - Materials Resource Registry and Repositories to disseminate and find data (**Working Group 1: MDCS, DSpace, MRR & MDF**)
  - Experimental and Computational data need for CALPHAD assessments (**Working Group 2: Experimental Data and Working Group 5: DFT**)
  - Ability to ease search and data re-use (**Working Group 4: NLP**)
- Need for outputs: Use-Cases
  - Co-base Superalloys for additive manufacturing
  - Shape-memory alloys (PdTi-based)
  - In-Situ Si composites/Thermoelectrics

Collaborations/Synergies

- Others at NIST
  - *Informatics*
    - *Working with ITL (Dima) to develop MDCS system*
    - *Working with TRC to develop ThermoML*
    - *Working NLP efforts by providing data to mine to develop terms*
  - *Use Cases*
    - *Co-base superalloys*
    - *Additive Manufacturing (Ni-base superalloys, steels, Ti6Al4V)*
  - *DFT Bench Marking*
  - *NIST Computational Tools*
    - *OpenCALPHAD*
    - *Materials Genome Toolkit*
  - *Development of CALPHAD assessments uncertainty quantification*
    - *Uncertainty of output (assessment)*
    - *Uncertainty of inputs (experimental data, computational data)*
    - *De-couple weighting of data for assessment process from the uncertainty of assessment*

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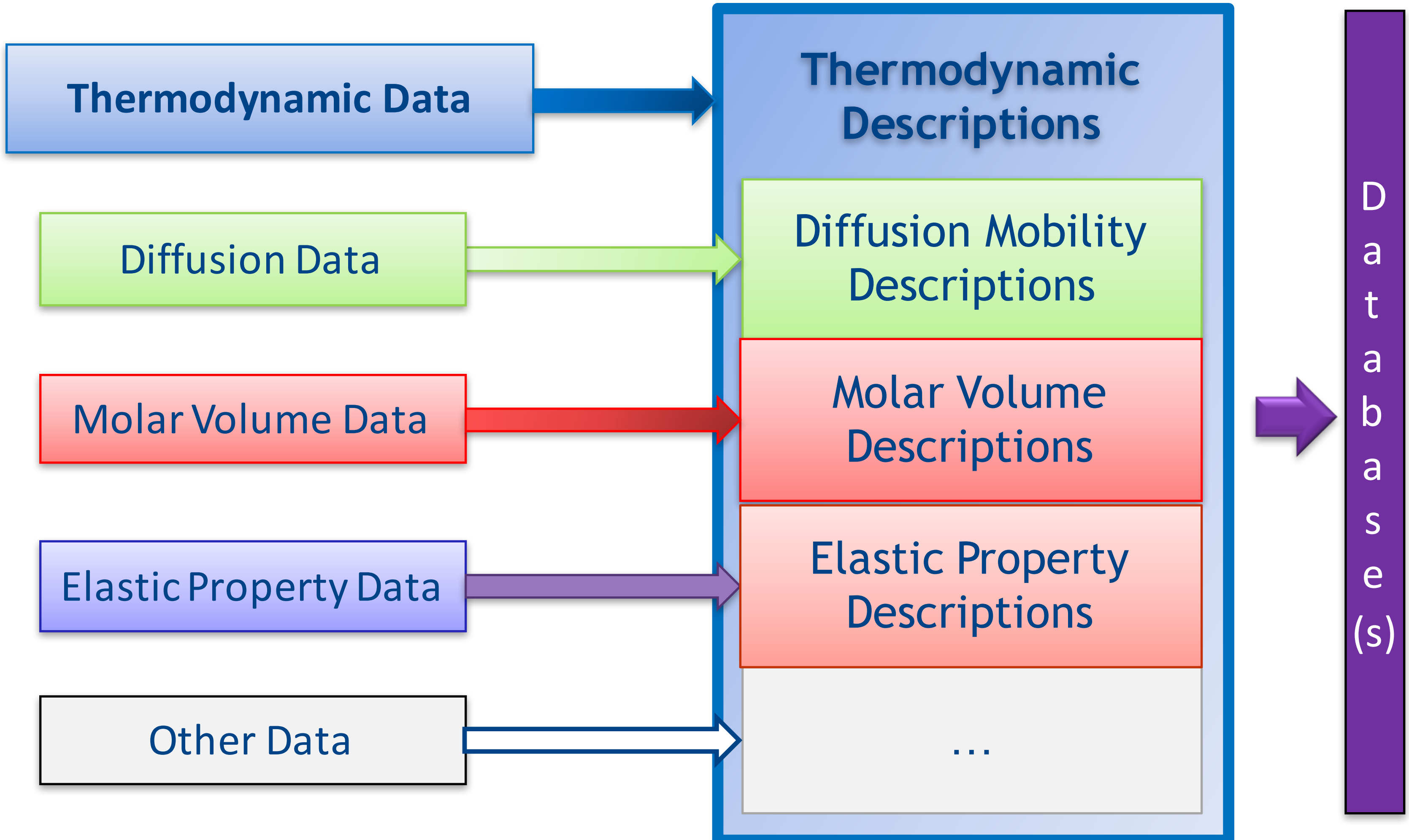
- Slides to help with discussion

Data Flow of CALPHAD Files

Evaluated Data Files | Functional Descriptions



Examples of Files for a CALPHAD Thermodynamic Assessment

Functional Description File Thermodynamics

- Elements: e.g. A,B
- Phases: e.g. FCC_A1 and BCC_A2 (crystal structure)
- Reference states used
- Software/version used
- Reference info
    - Bibliographic info
    - DOI link
- Contributor info
    - Name
    - E-mail
- User Comments
- Links to other files

Evaluated Data Files Thermodynamics (POP)

- Link to associated TDB file
- Elements: e.g. A,B
- Phases: e.g. FCC_A1 and BCC_A2 (crystal structure)
- Software/version used (e.g. TC-PARROT, ver S)
- Reference info for data
    - Bibliographic info
    - DOI link
- Author info
    - Name
    - Reference info
        - Bibliographic info
        - DOI link
- Contributor info
    - Name
    - E-mail
- User Comments
- Links to other files

Auxiliary Files (e.g. EXP, TCM)

- Link to POP and/or TDB
- Elements
- Phases
- Reference info
- Author
- User
- Links to other files

Note: Thermo-Calc based file extensions used, but information on file types should also be included

Examples of Files for a CALPHAD: Diffusion Mobility Assessment

Database files

Thermodynamic Description

Link to TDB file or reference

Diffusion Mobility Description

- Elements: e.g. A,B
- Phases: e.g. FCC_A1 and BCC_A2 (crystal structure)
- Software/version used
- Reference info
  - Bibliographic info
  - DOI link
- Contributor info
  - Name
  - E-mail
- User Comments
- Links to other files

Evaluated Data Files (e.g.DOP)

- Link to associated TDB file
- Elements: e.g. A,B
- Phases: e.g. FCC_A1 and BCC_A2 (crystal ctructure)
- Software/version used (e.g. TC-PARROT, ver S)
- Reference info for data
  - Bibliographic info, DOI link
- Author info
  - Name
  - Reference info
    - Bibliographic info, DOI link
- Author info
  - Name, e-mail
- User Comments
- Links to other files

MACRO/Script Files (e.g. to run simulations , DCM)

- Elements
- Phases
- Reference
- Author
- Links to other files (grid data, start values)
- User comments

Auxiliary Data Files (e.g. *.EXP)

- Link to POP and/or TDB
- Elements
- Phases
- Reference info
- Author
- Links to other files
- User comments

Note: Thermo-Calc based file extensions used, but information on file types should also be included

https://materialsdata.nist.gov/dspace/xmlui/

Login

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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

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Customized DSpace repository for materials
- ➢ Enables sharing of a variety of data types, including text, images, and video

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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.2005.07.016

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.

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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, Keith Hammond and Karen Denike for their experimental support.

Data files

Files in this item

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

View/Open

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

View/Open

The following license files are associated with this item:

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This item appears in the following Collection(s)

- Diffusion Data

Except where otherwise noted, Universal

Related items

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

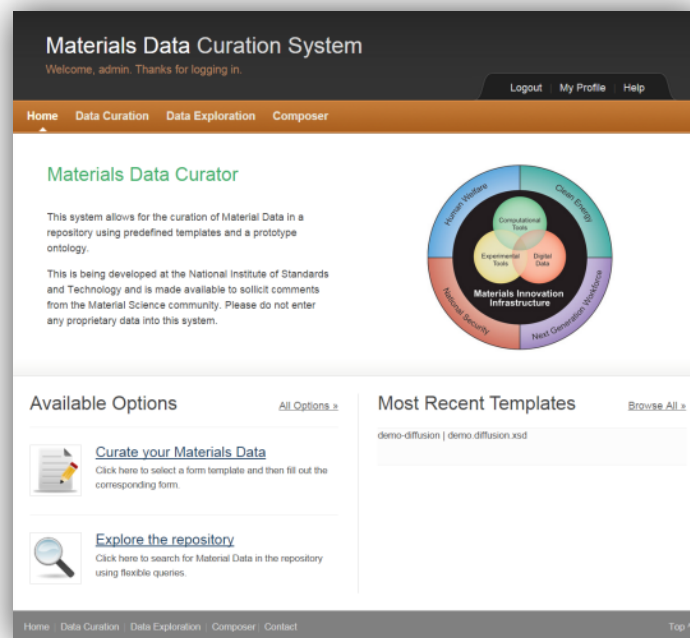
Further Studies on the Nickel-Aluminum System. I. The β-Ni2Al3 Phase Fields
Taylor, A; Doyle, N.J. (1972-01-31)
New lattice parameter and density results have been obtained for alloys in the fl-NiA1 and 6-Ni2A13 phase fields of the nickel-aluminum system. The lattice parameter of the fl-NiAl phase (CsCl-type) 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 ...

Material Data Curation System (MDCS)

- **Need**
  - Difficult to
    - Combine data from multiple sources
    - Understand and reuse existing data
    - Find associated metadata
    - Transform data into new formats
- **Objectives**
  - Facilitate collection, use, and reuse of materials data
  - Provide needed informatics infrastructure to enable High Throughput Experimentation (HTE)

https://github.com/usnistgov/MDCS



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Nanomechanical Properties Group

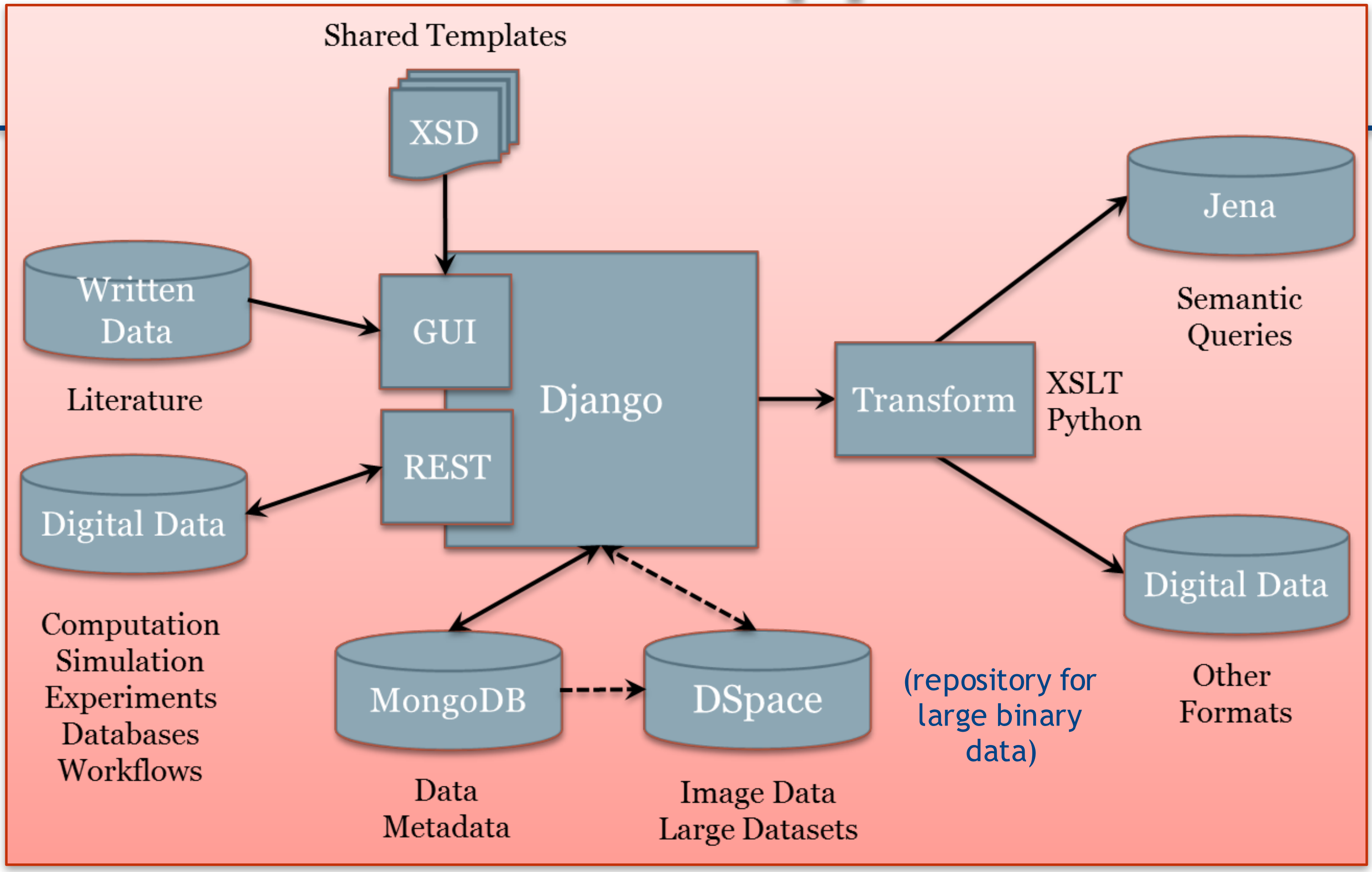
Office of Data and Informatics

Polymers and Complex Fluids Group

Mechanical Performance Group

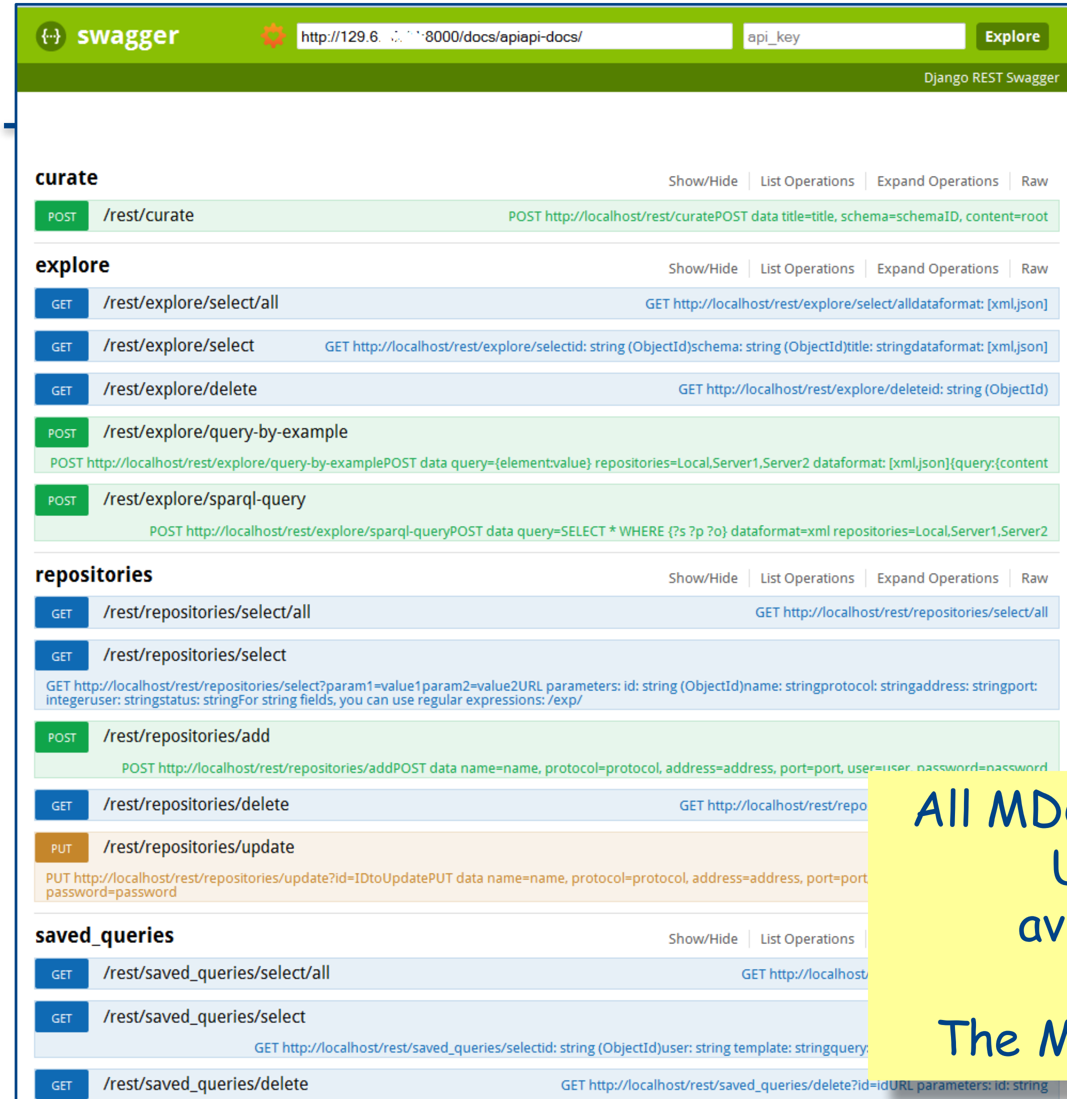
Alden Dima, NIST

The MDCS Approach



- Web-based: Python/Django/MongoDB, REST API, XML-based, SPARQL queries
- Store data in XML-based templates
- Store, manage, & compose templates
- Spreadsheet input

MDCS REST API



All MDCS functions available via the User Interface are also available via the REST API

The MDCS can be fully automated

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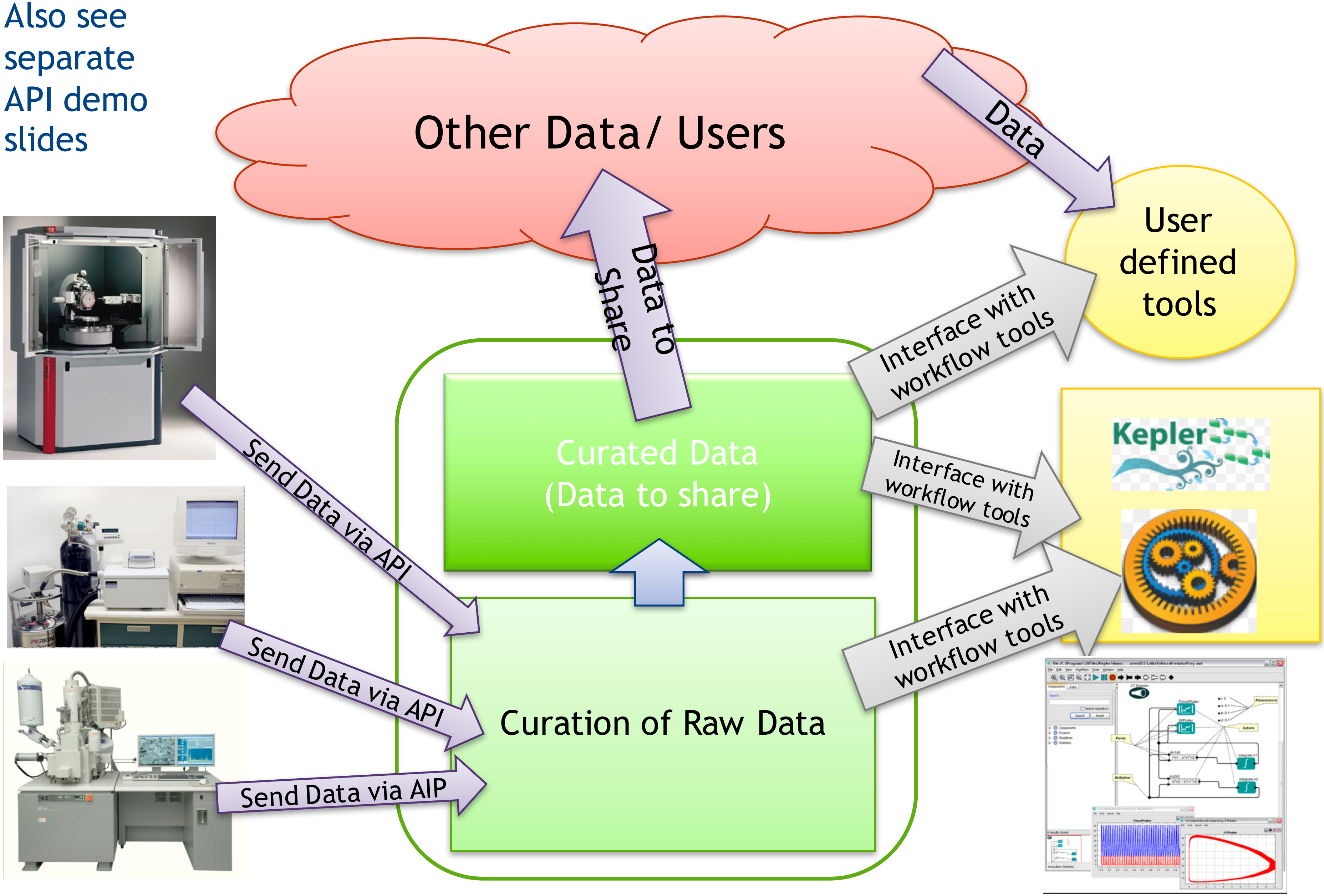
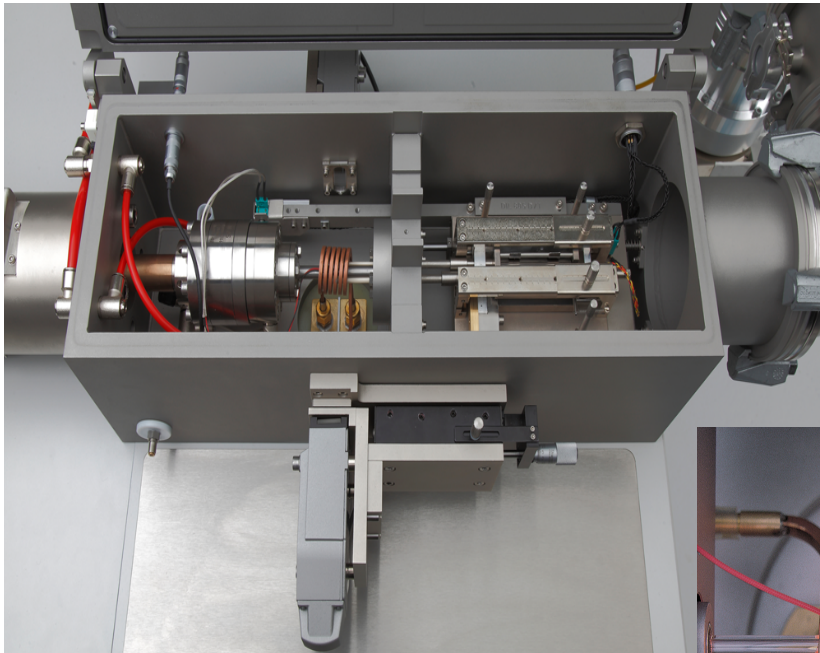
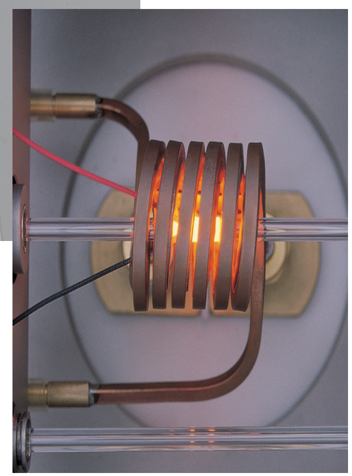
Materials Data Curation

Also see separate API demo slides

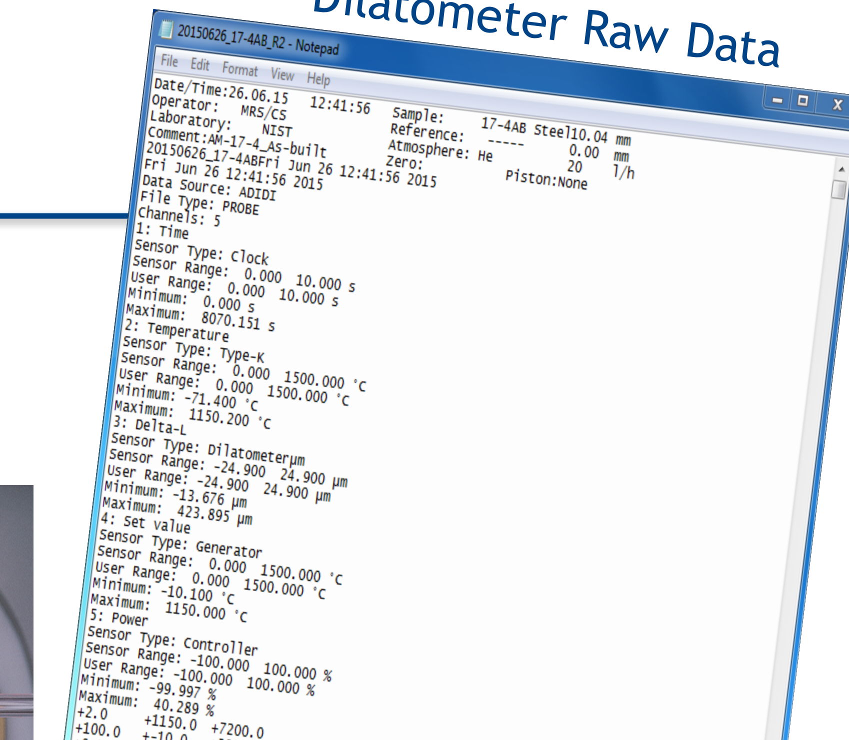


Dilatometer





Dilatometer Raw Data



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Comment:AM-17-4_As-built         Zero:            Piston:None
20150626_17-4ABFri Jun 26 12:41:56 2015
Fri Jun 26 12:41:56 2015
Data Source: ADIDI
File Type: PROBE
Channels: 5
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Sensor Type: Clock
Sensor Range:   0.000   10.000 s
User Range:   0.000   10.000 s
Minimum:   0.000 s
Maximum:   8070.151 s
2: Temperature
Sensor Type: Type-K
Sensor Range:   0.000   1500.000 'C
User Range:   0.000   1500.000 'C
Minimum: -71.400 'C
Maximum:   1150.200 'C
3: Delta-L
Sensor Type: Dilatometerµm
Sensor Range: -24.900   24.900 µm
User Range: -24.900   24.900 µm
Minimum: -13.676 µm
Maximum:   423.895 µm
4: Set value
Sensor Type: Generator
Sensor Range:   0.000   1500.000 'C
User Range:   0.000   1500.000 'C
Minimum: -10.100 'C
Maximum:   1150.000 'C
5: Power
Sensor Type: Controller
Sensor Range: -100.000   100.000 %
User Range: -100.000   100.000 %
Minimum: -99.997 %
Maximum:   40.289 %
+2.0       +1150.0     +7200.0
+100.0     +-10.0      +300.0
+0.0       +0.0        +0.0
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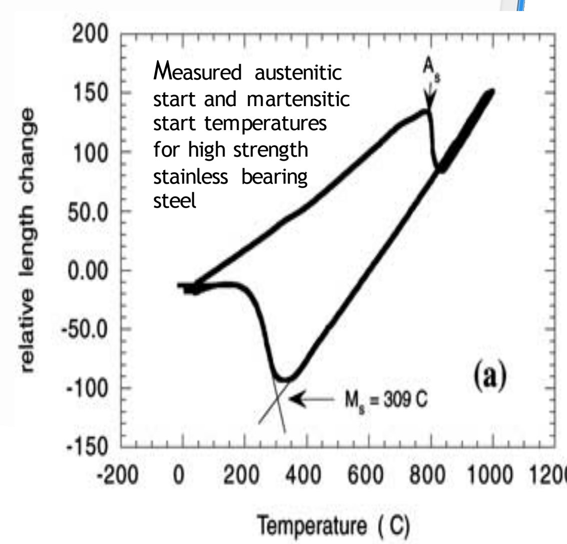
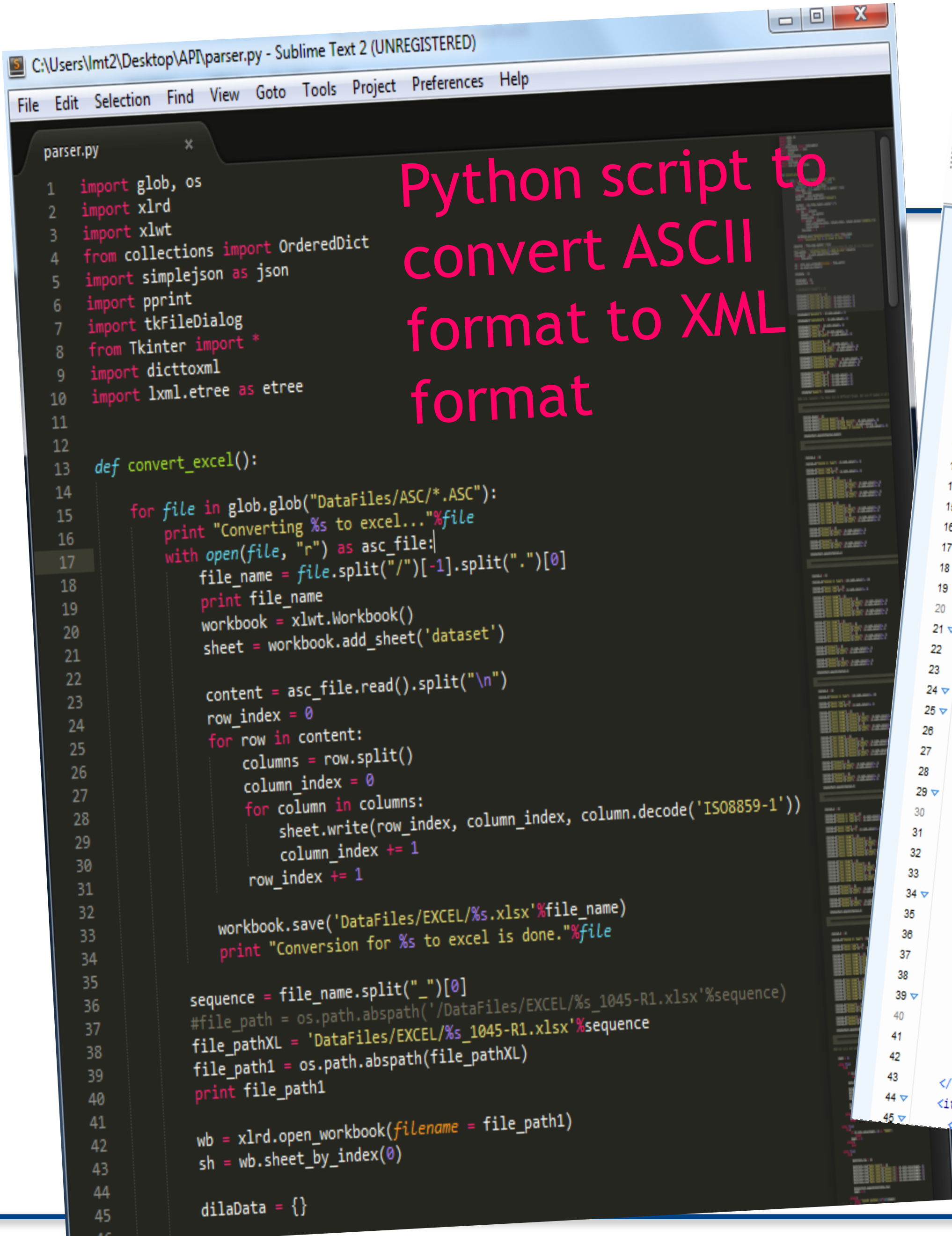
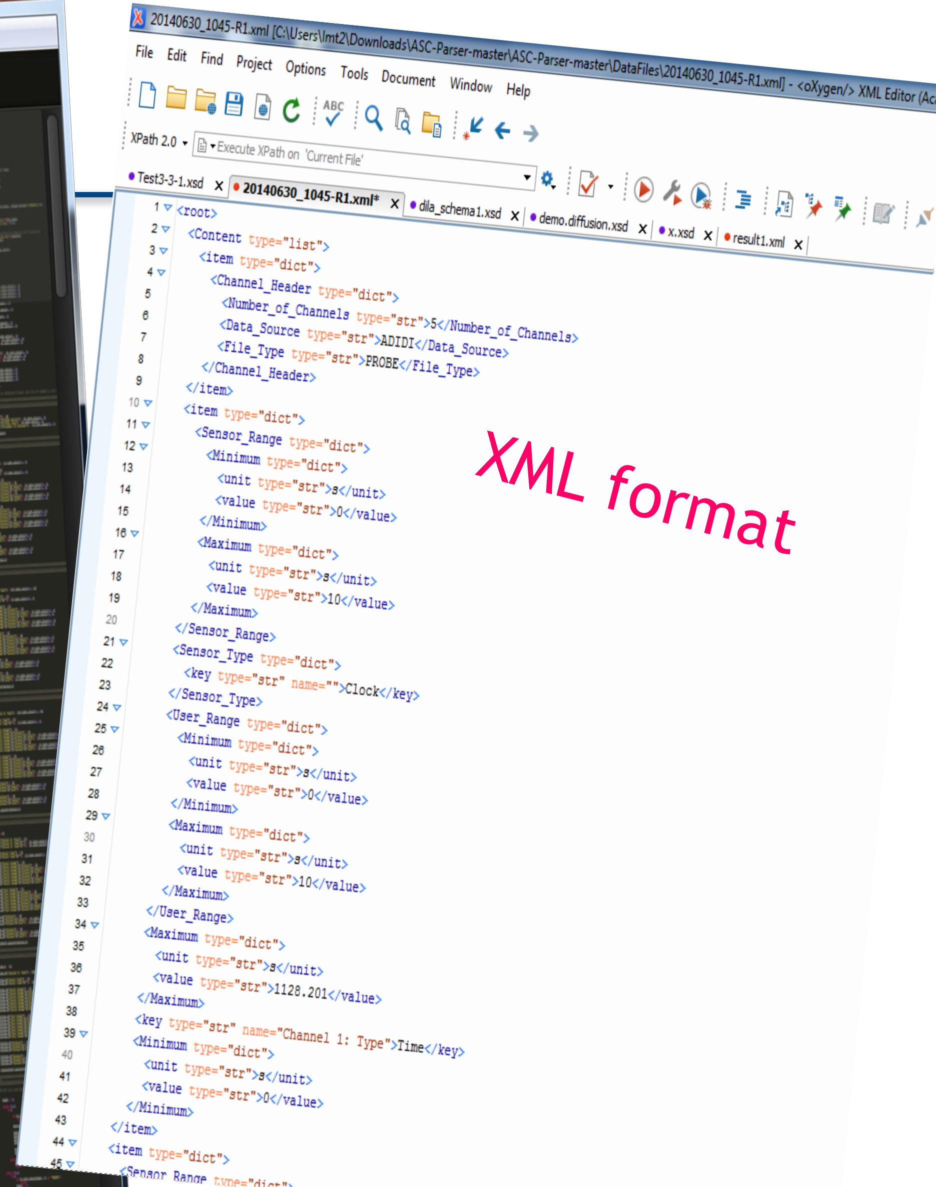


Raw Data from a dilatometer: Length vs Temperature



Python script to convert ASCII format to XML format



XML format

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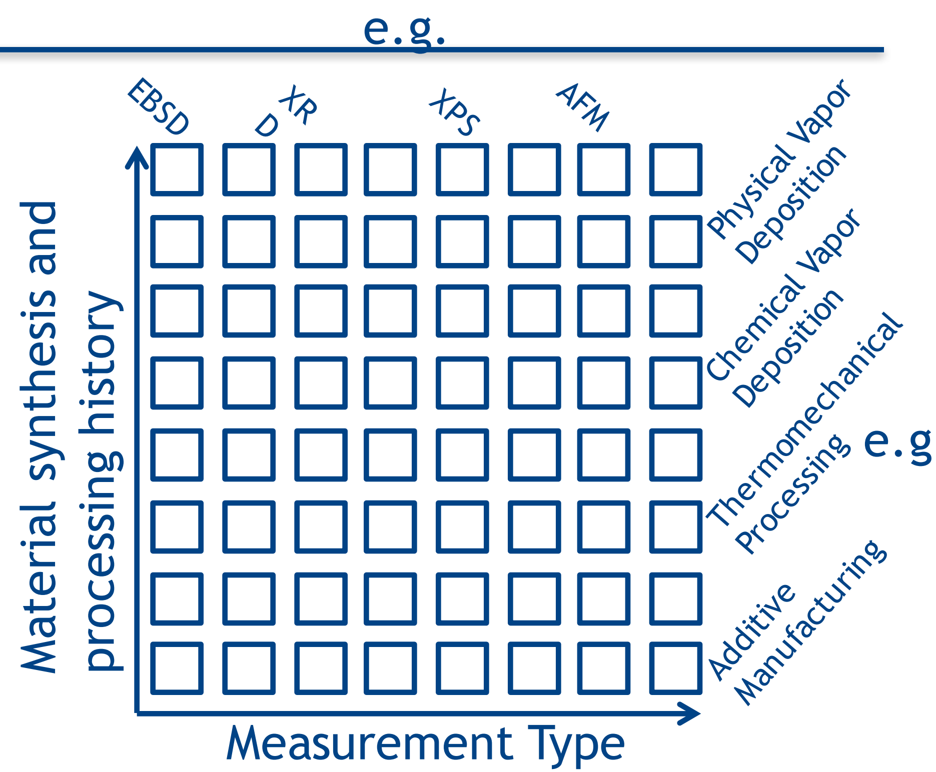
Need: Modular Data Models

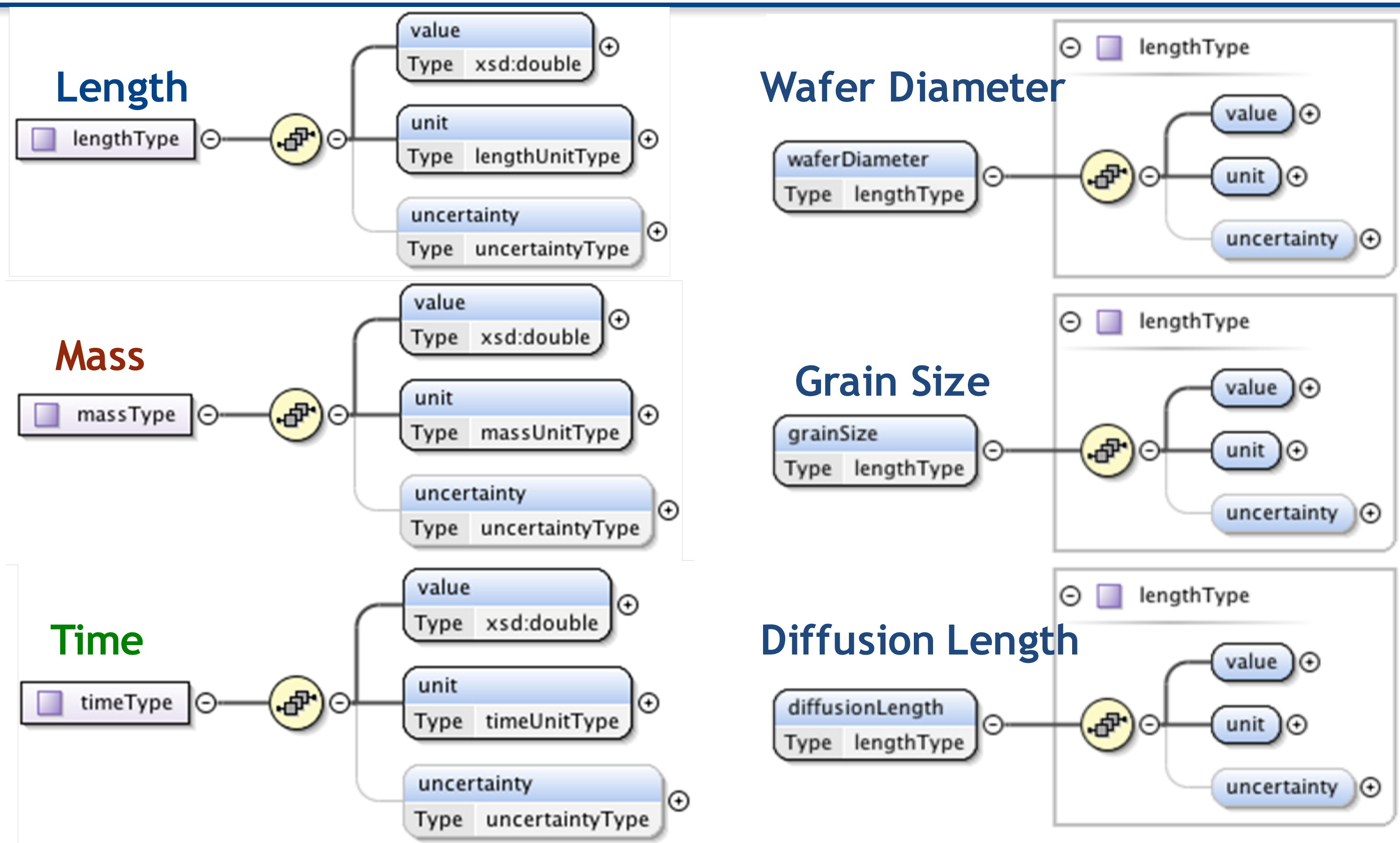
- **Data Model Definition**
  - Defines the structure of data and metadata associated with the measurement or synthesis
- **Modularity**
  - Via the MDCS composer assemble modules for your workflow
  - Modify as modules needed
- **Not a standard**
  - Flexible data structures
  - Common reusable types
  - Domain modules



Foundation:
- Shared Types
  - E.g. Chemical Substance
- Physical Quantities
  - E.g. Pressure

Reusable Data Types

Base Types



Physical Quantities: SP811

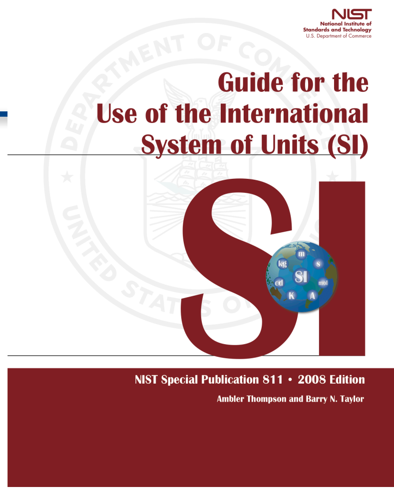
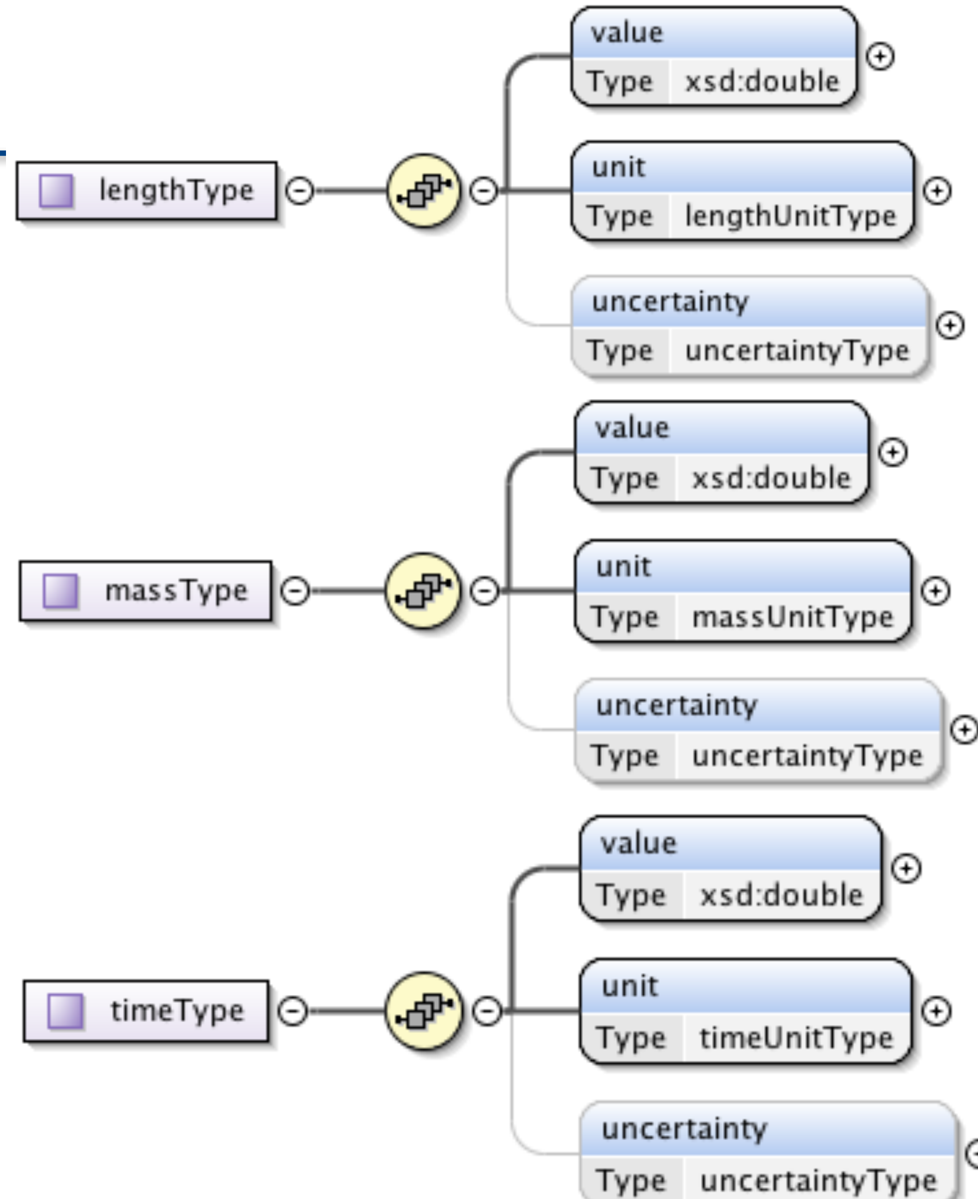
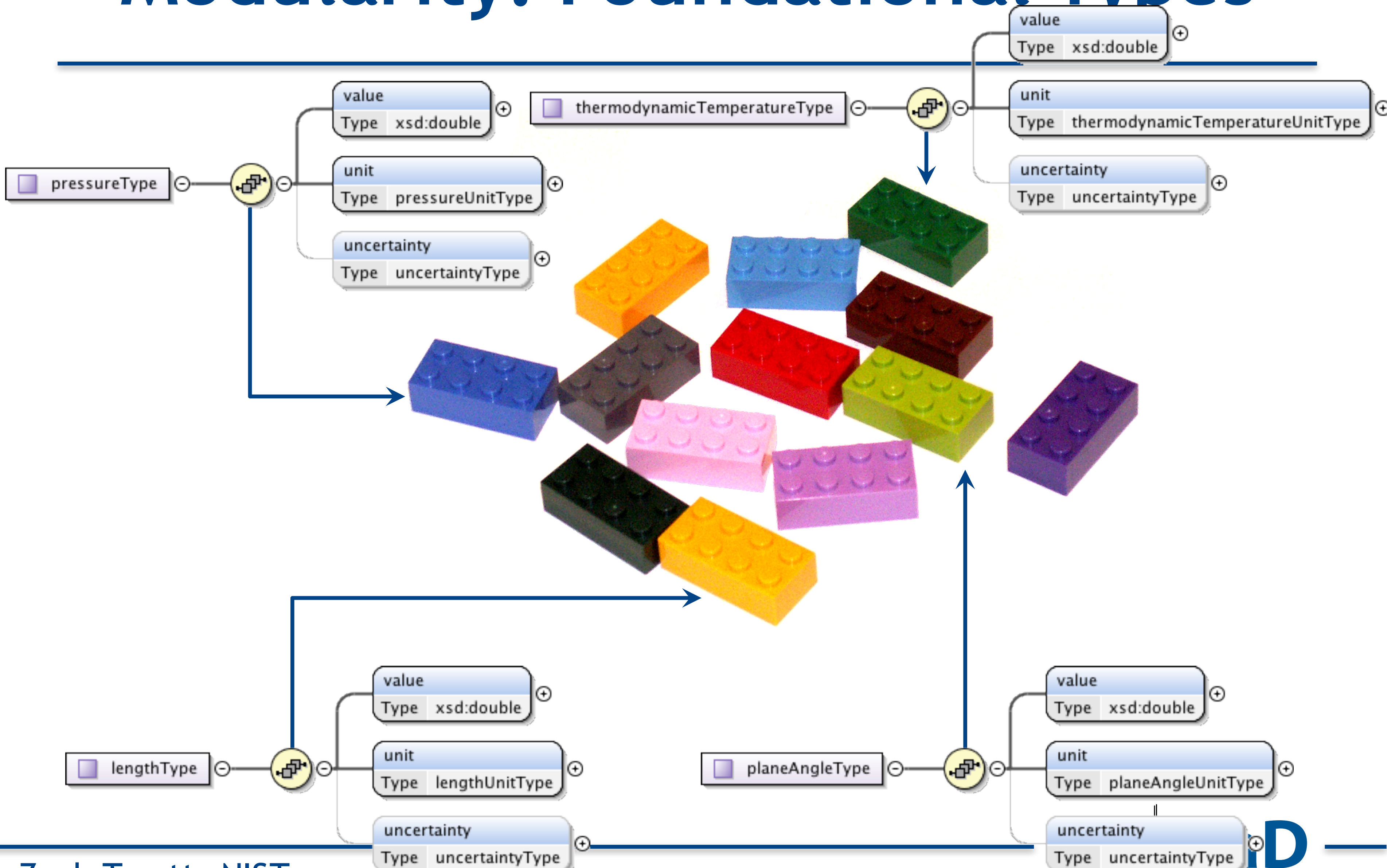


Table 1. SI base units

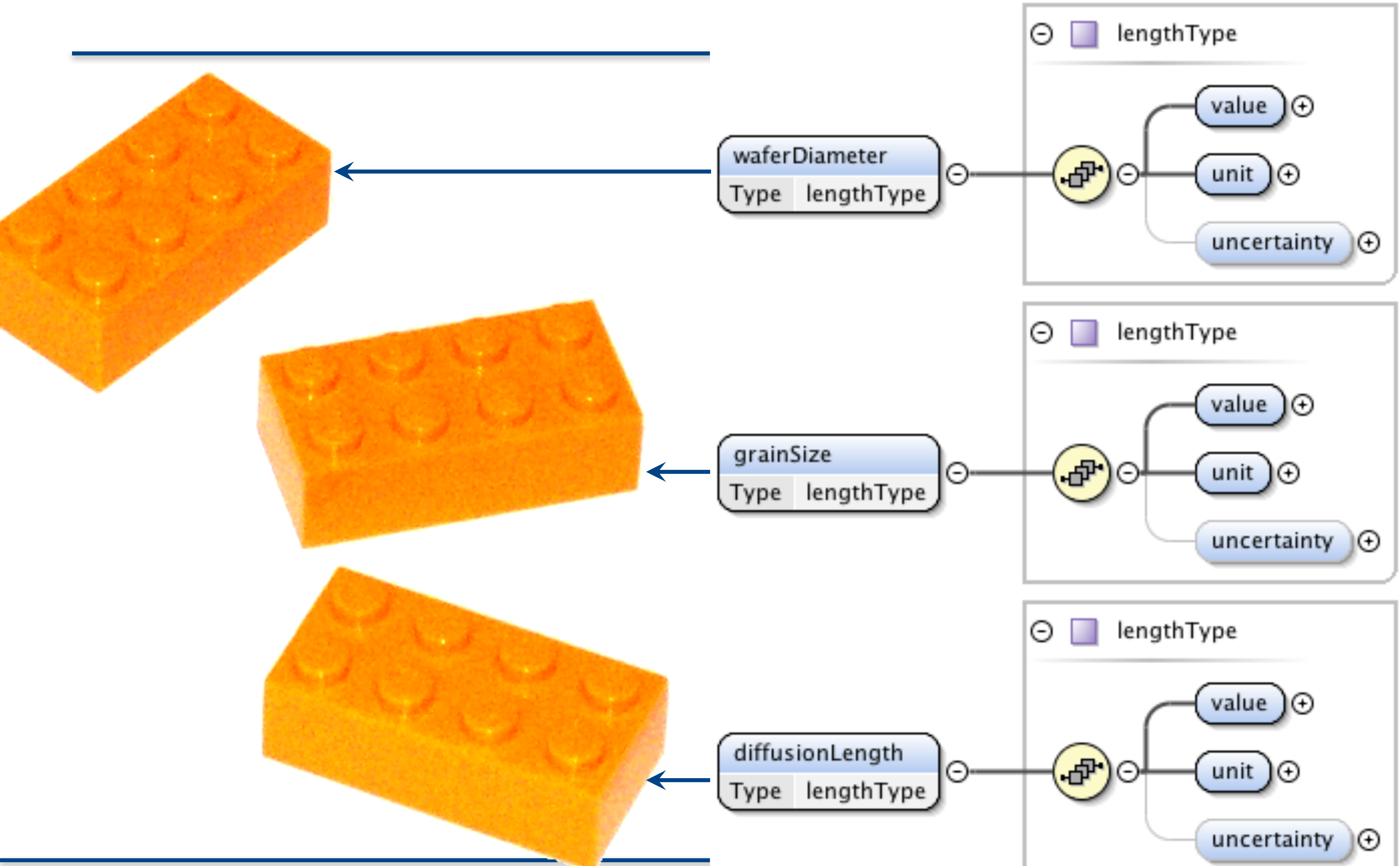
Base quantity
length
mass
time
electric current
thermodynamic temperature
amount of substance
luminous intensity



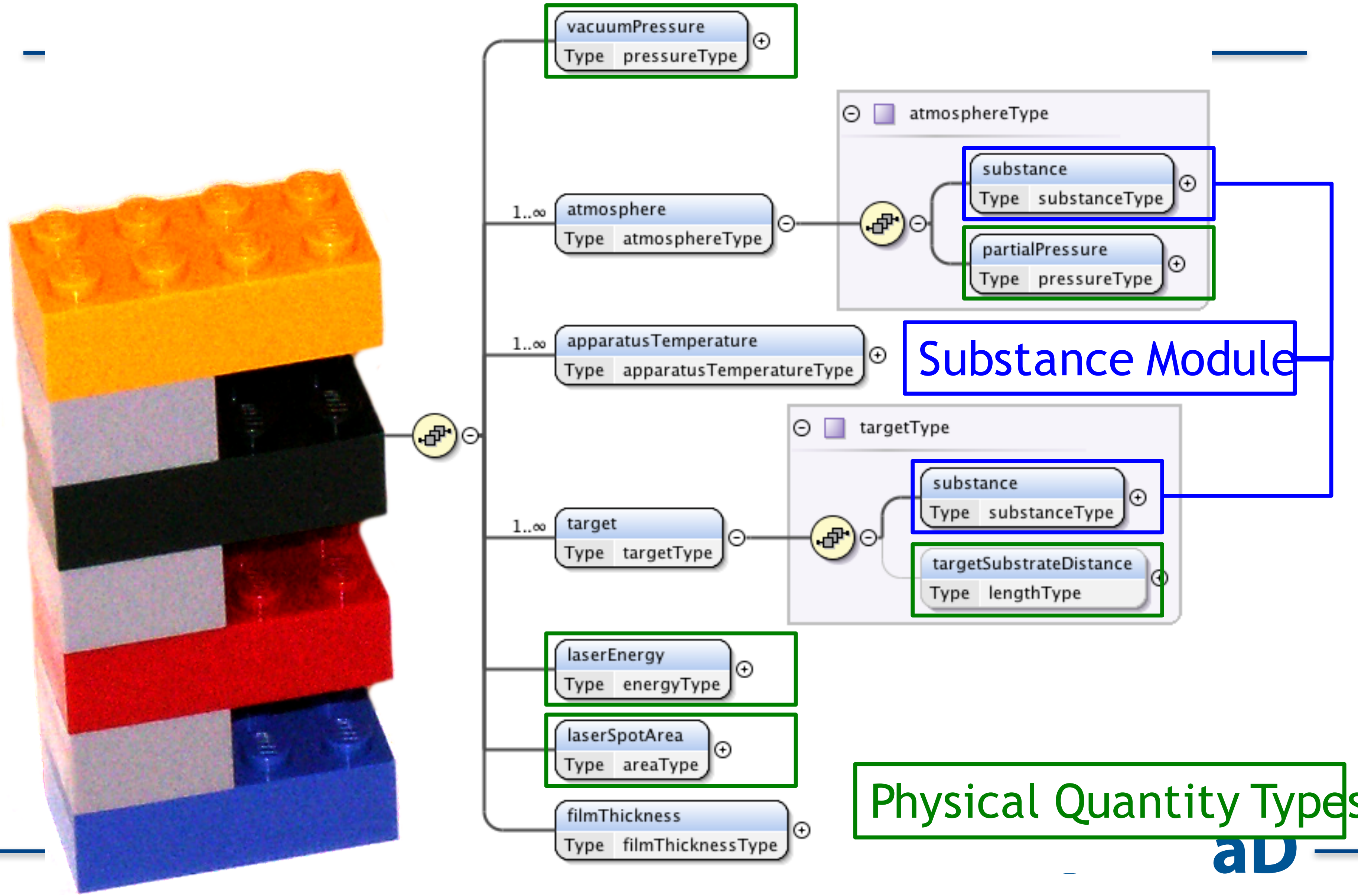
Modularity: Foundational Types



Modularity: Foundational Types

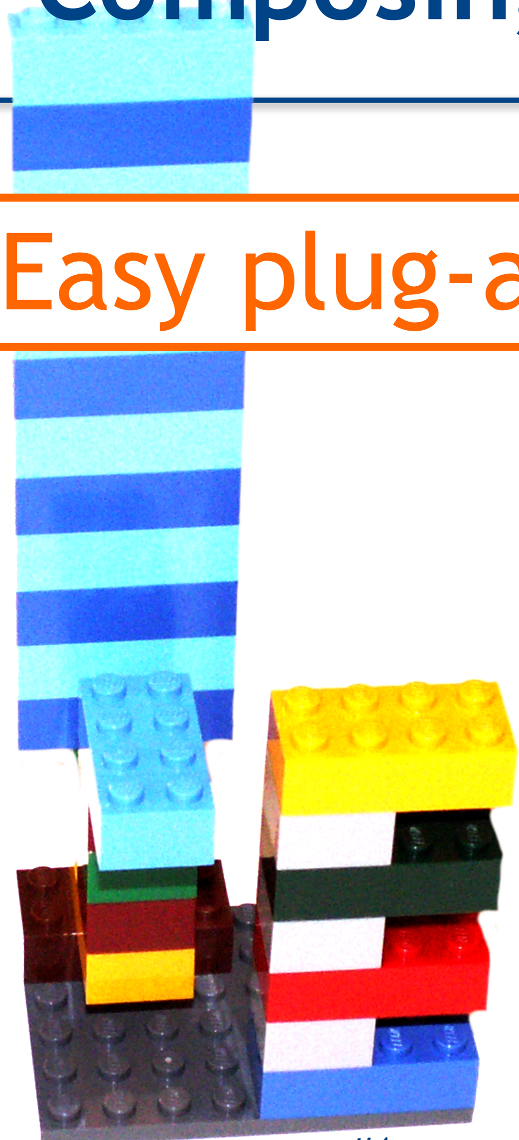


Modularity: Synthesis Example

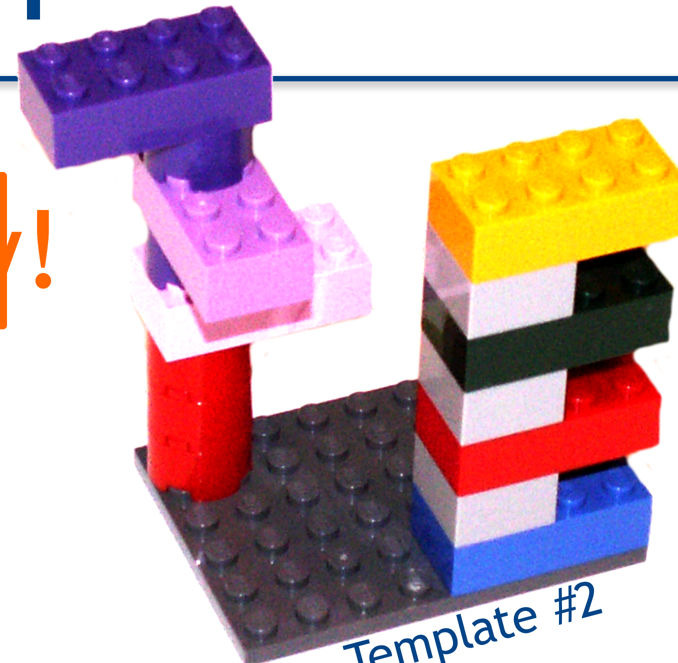


Composing a Template in MDCS:

Easy plug-and-play!



Template #1



Template #2

Primary Goal:

- **Reduce startup cost:** time required to create Template

Warning: Side effects include standardization through popularity and ease of use

Examples of CALPHAD Data

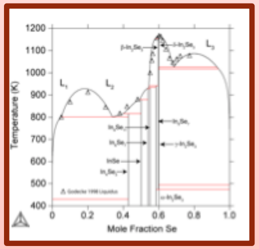
For each assessment: Evaluated data file (e.g. POP, DOP)
Functional descriptions for phase quantity (e.g. TDB)

- Emphasis on binary and ternary data to predict multicomponent properties
- Data can be experimental or computational.

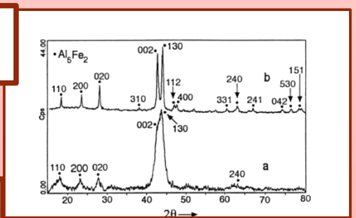
1-D (Points)

Melting Temperatures

Critical Temperatures (Phase Changes)



Lattice Parameters



Heat of Formations

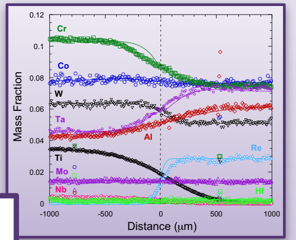
Phase fractions and compositions

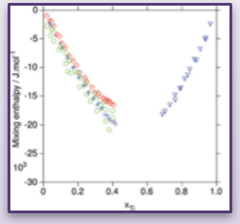
Tracer Diffusivities

Activation energies

2-D (Lines)

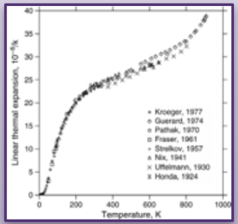
Composition Profiles





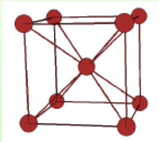
Heat Capacities

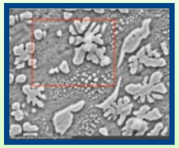
Enthalpies of mixing



3-D

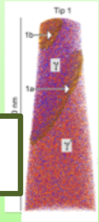
Crystal structures





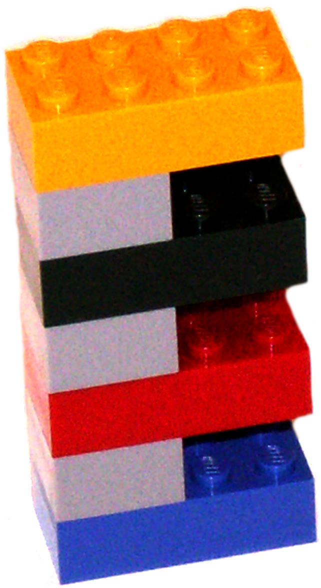
Micrographs/Morphologies

3-D Atom probe Tomography

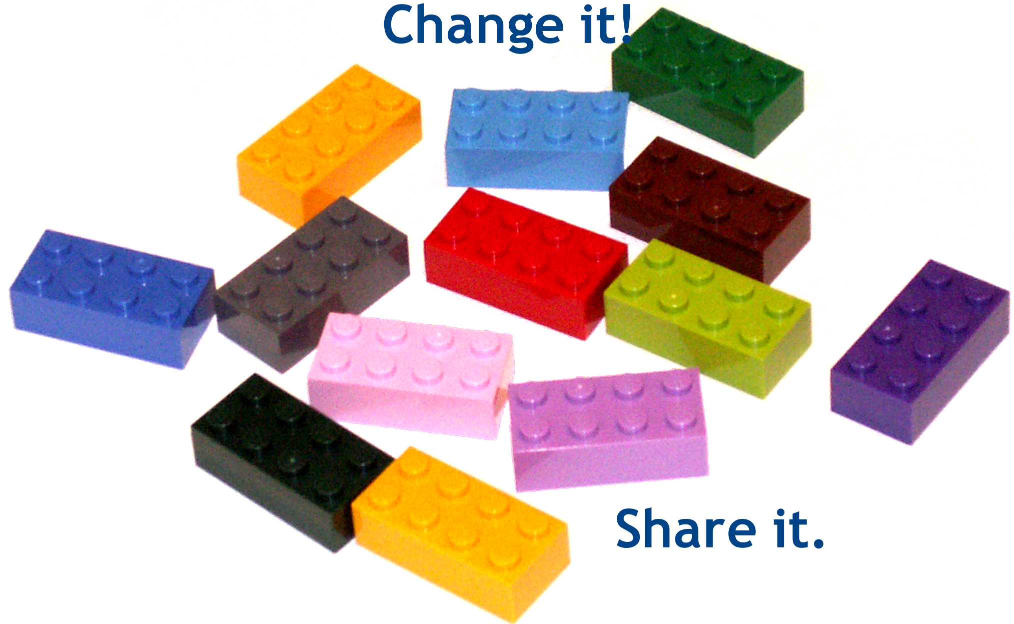


Not a standard

Module not quite right?



Change it!



Share it.

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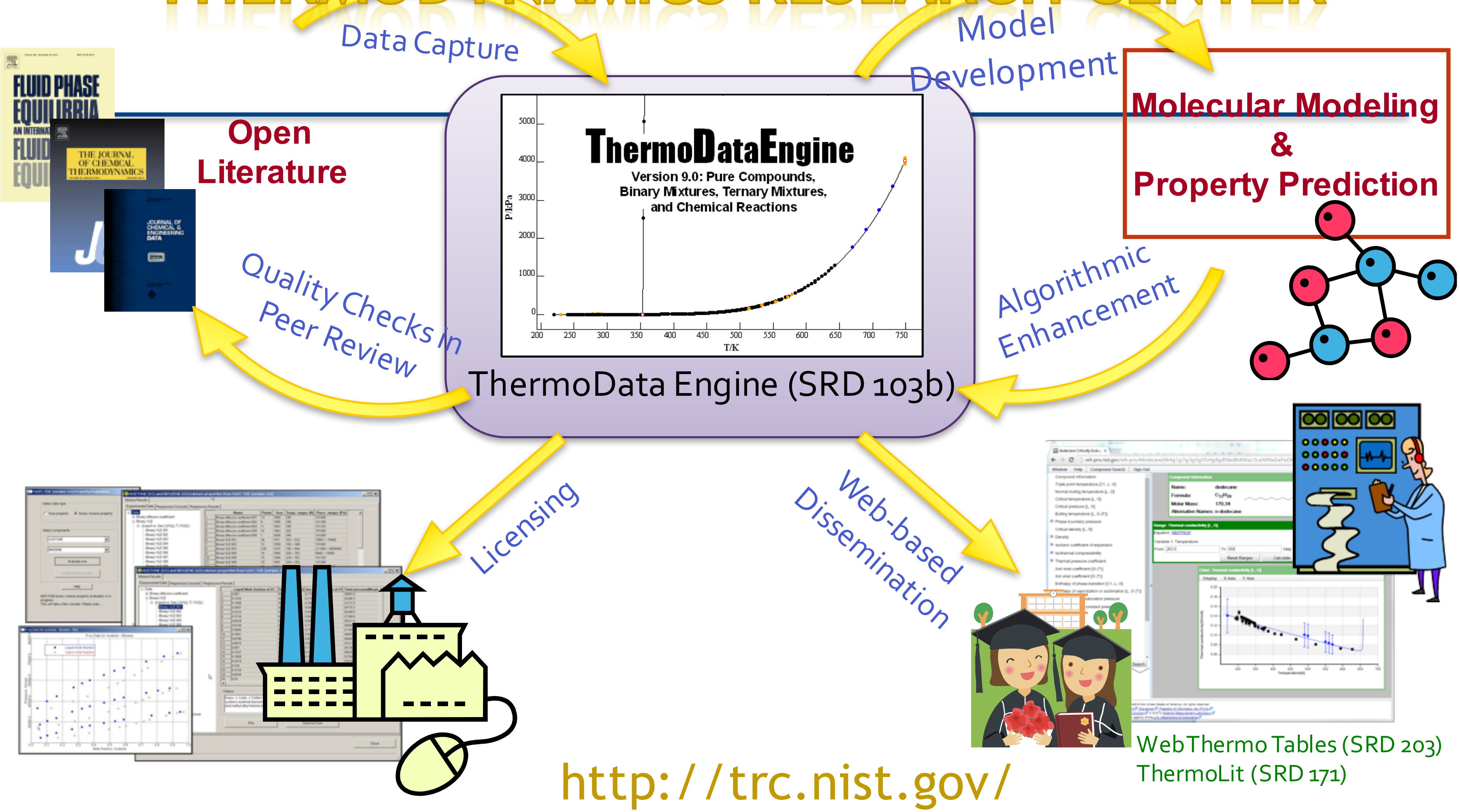

- Expanding to metallic systems
- Initial focus on phase equilibria data and thermochemical property data.

CHiMaD