Data Needs for the MGI at NIST

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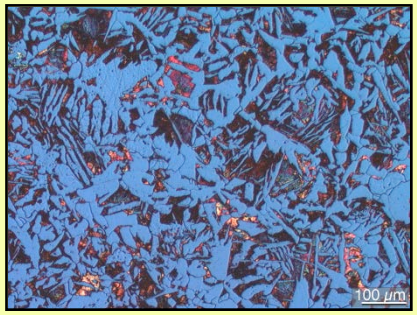
Why a Materials Genome Initiative?

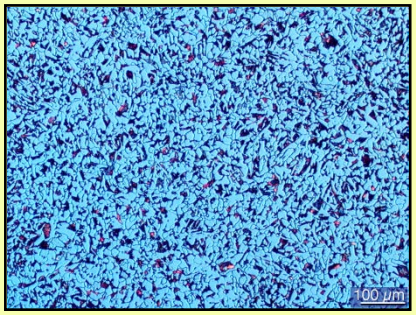
Materials Are Complicated Systems
Modeling is a Challenge

- Advanced materials often consist of several components (generally, $n > 5$) and multiple phases.
- The phases present change as a function of processing and service conditions.

Material A cooled from 300 °C



Material A cooled from 800 °C



Microstructures consist of mixtures of multiple phases.

A finer microstructure is obtained at the higher temperature.

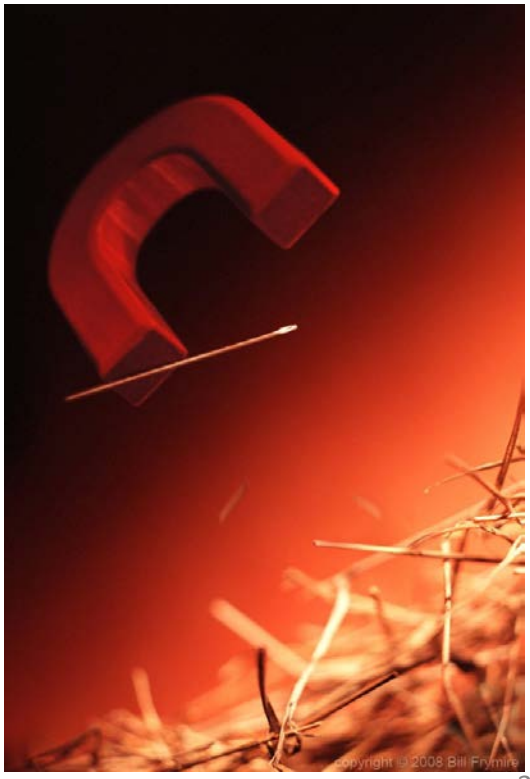
The finer microstructure results in a much stronger alloy

Why Materials Design?

Materials development is a “needle in haystack” problem

- If an empirical approach is taken to develop new materials, number of possible compositions to evaluate is overwhelming.
  - e.g., superalloys, which often contain 12 components, if one only considers the *current composition ranges* the number of compositions to investigate exceeds $1x10^8$

The right tools:
MGI ?



Materials Genome Initiative

A genome is a set of information encoded in the language of DNA that serves as a blueprint for an organism's growth and development. The word genome, when applied in non-biological contexts, connotes a fundamental building block toward a larger purpose.

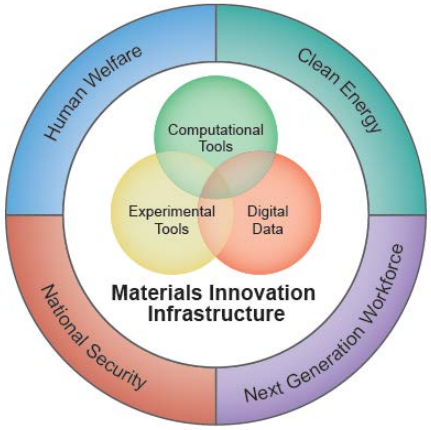


Figure 3: Initiative overview

- The Materials Genome Initiative is a new, multi-stakeholder effort to develop an infrastructure to accelerate advanced materials discovery and deployment in the United States. Over the last several decades there has been significant Federal investment in new experimental processes and techniques for designing advanced materials. This new focused initiative will better leverage existing Federal investments through the use of computational capabilities, data management, and an integrated approach to materials science and engineering.

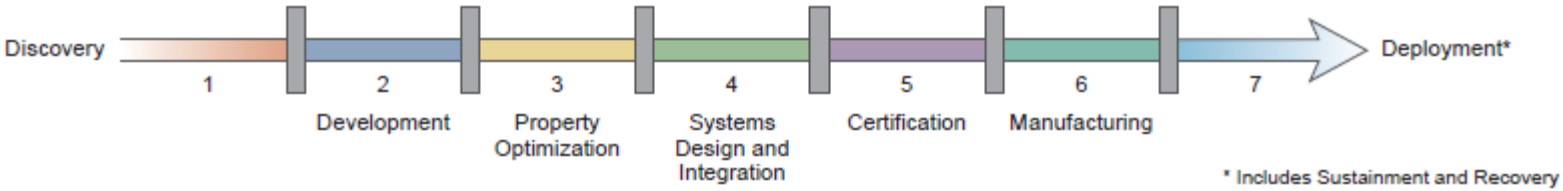


Figure 1: Materials development continuum

NIST and the MGI

MGI Vision

The Materials Genome Initiative (MGI) will significantly reduce the time for materials discovery, optimization, and deployment through the promotion of a new R&D paradigm in which powerful computational modeling, simulation, and analysis will decrease the reliance on time-consuming, expensive, physical experimentation.

NIST Role

NIST will provide the measurement and standards infrastructure needed to realize the MGI.

Implementation

- **NIST will work with stakeholders in industry, academia and government to develop:**
- **Standards and tools for the representation and interoperability of materials data, whether from simulation or experiment**
- **Techniques and standards for the interoperation of modeling systems operating at multiple length and time scales**
- **Techniques and tools for the quality assessment of models, simulations, and the materials data generated from them.**

These techniques, standards, and tools will be developed through implementations and enhancements of existing NIST expertise and methods that provide materials property data and related software to the research community. Initial efforts will focus on two pilot areas: (a) structural metallic alloys of interest to the aerospace and transportation sectors, and (b) advanced composites of interest in transportation, energy, and electronics.

Expected Outcomes

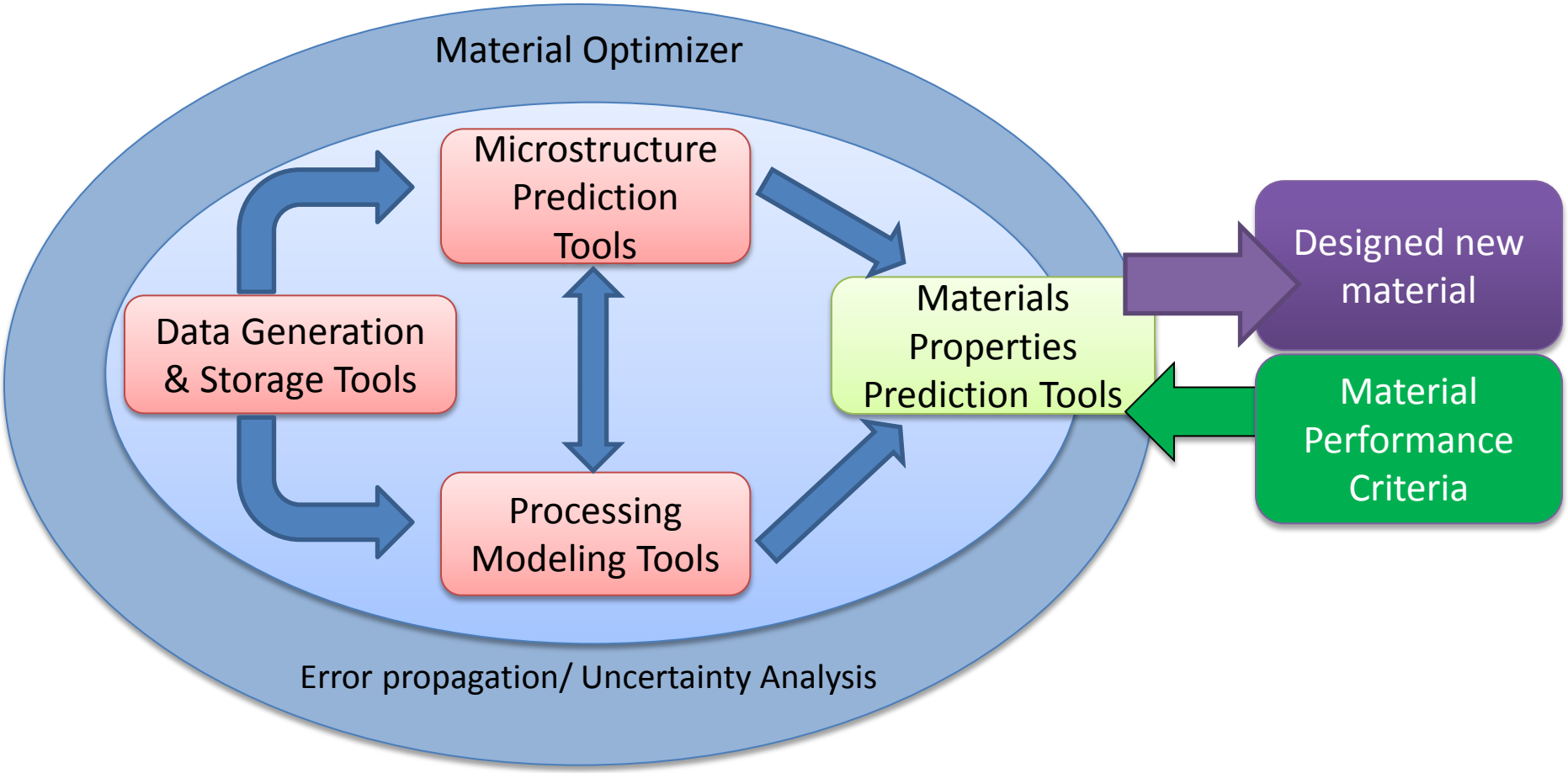
Improved access to data/models/simulations

Easier composition of models operating at differing length and time scales

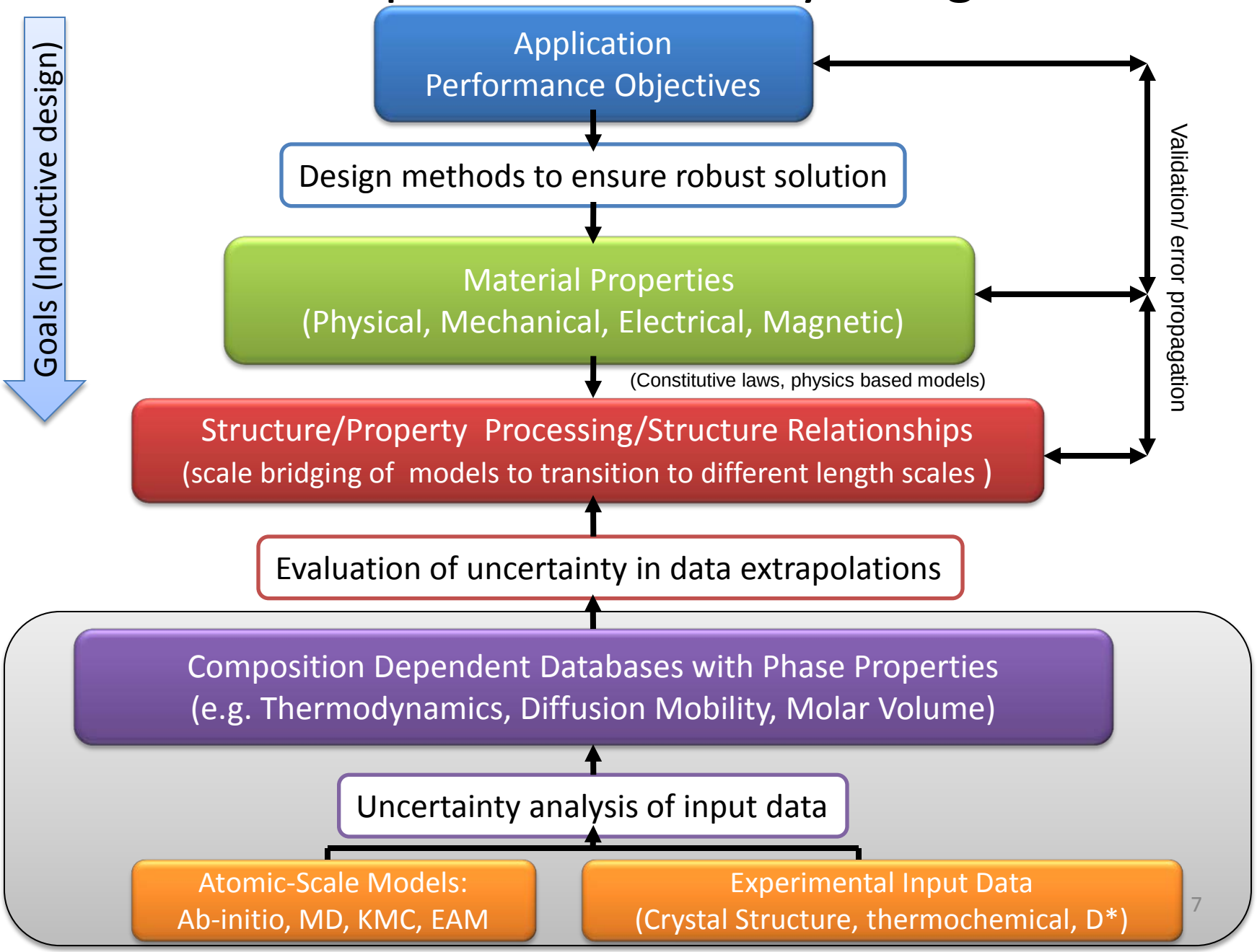
Improved model reliability and confidence in results

Reduced barriers to adopting state-of-the-art methods and techniques

Materials Genome: Goal

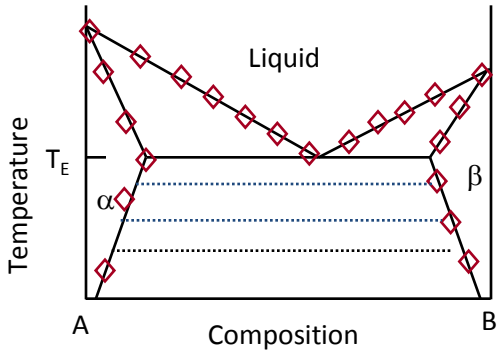


Roadmap for Materials by Design

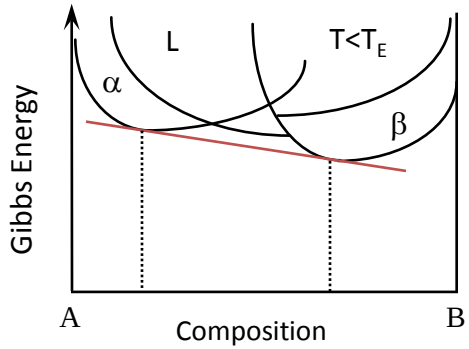


Original CALPHAD Approach

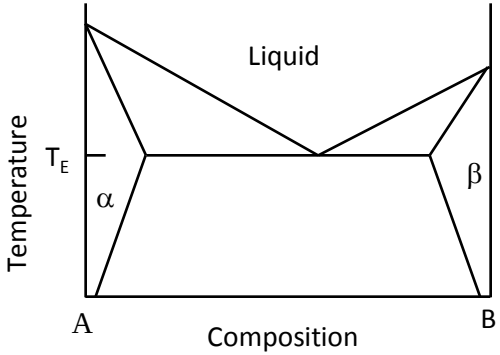
Experimental phase diagram and thermochemical data



Determine Gibbs energy functions for each phase: $G = f(x,T,P)$



Calculated phase diagram



$$G^{\phi} = G^{0} + G^{ideal} + G^{excess}$$

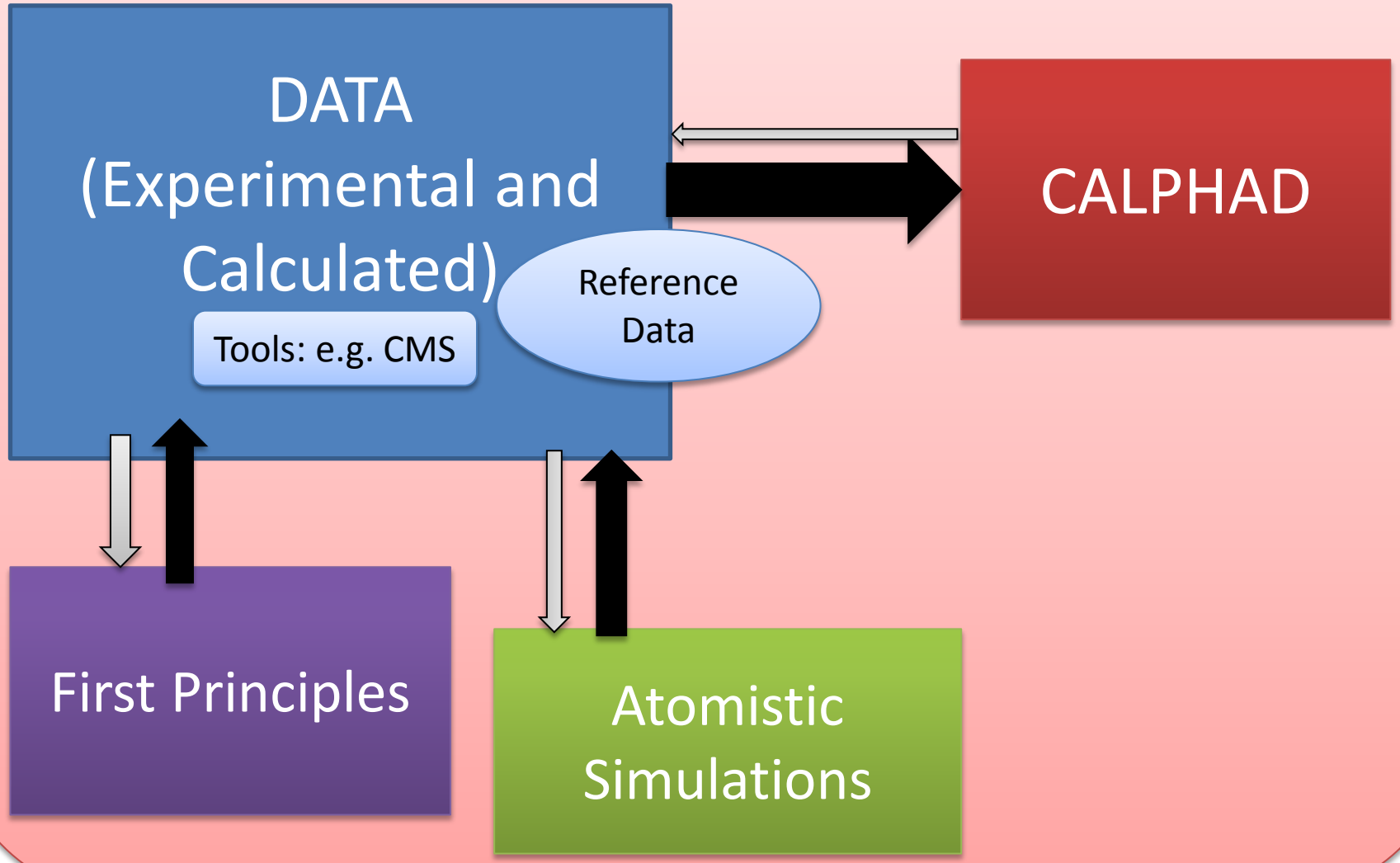
Binaries ⇨ Ternaries ⇨ Quaternaries ⇨ n^{th} Order Systems

True quaternary compounds are rare in metallic systems

⇨Assessment of ternary systems is usually sufficient for the description of a multicomponent system

⇨Same methodolgy can be applied to the description of other property data

Data Generation & Storage Tools



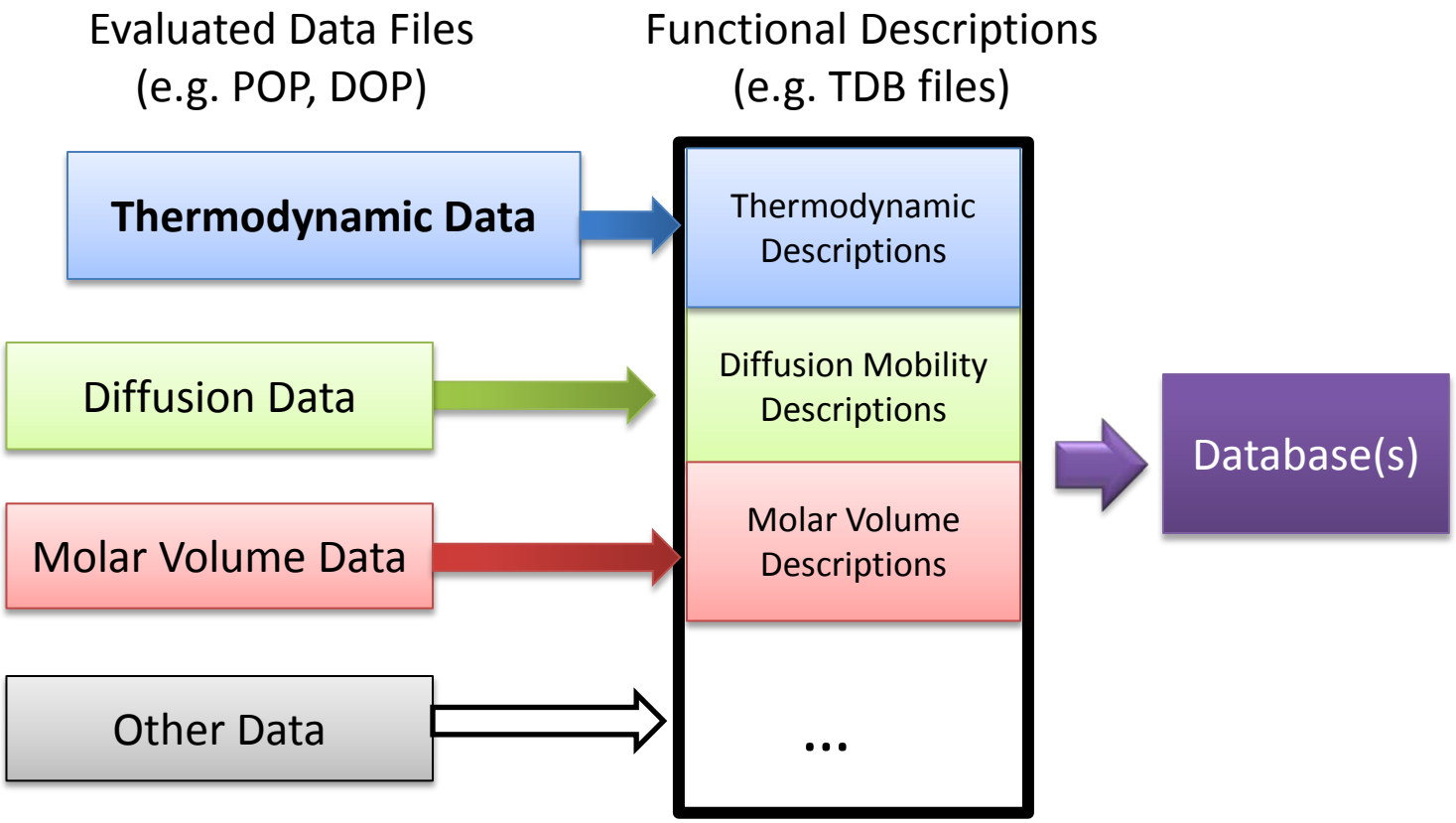
Current MGI Needs

- Need a flexible and evolving repository for both calculated and measured data.
  - Materials and crystal structures need to have unique identifications.
- Need repositories for CALPHAD-based, atomistic simulations and first-principles files.
- Need general repository for data
  - Initial focus on data needed for the development of CALPHAD descriptions

Linkage of CALPHAD Descriptions

Gibbs energy	$G = g(T, P, N_i)$
Entropy	$S = -\left(\frac{\partial G}{\partial T}\right)_{P,N_i}$
Enthalpy	$H = G - T\left(\frac{\partial G}{\partial T}\right)_{P,N_i}$
Heat capacity	$C_P = -\left(\frac{\partial^2 G}{\partial T^2}\right)_{P,N_i}$
Chemical potential	$\mu_i = -\left(\frac{\partial G}{\partial N_i}\right)_{P,T,N_{j\neq i}}$
Volume	$V = -\left(\frac{\partial G}{\partial P}\right)_{T,N_i}$
Thermal expansion	$\alpha = \frac{1}{V}\left(\frac{\partial^2 G}{\partial P \partial T}\right)_{N_i}$
Isothermal compressibility	$\kappa = -\frac{1}{V}\left(\frac{\partial^2 G}{\partial P^2}\right)_{T,N_i}$
Bulk modulus	$K = \frac{1}{\kappa}$
Intrinsic diffusivity	${}^{i}D_{jk} = N_j M_j \frac{\partial \mu_j}{\partial N_k}$

Structure of CALPHAD Database Files



Examples of Files for a CALPHAD Thermodynamic Assessment

Functional Description File Thermodynamics: TDB file

- 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

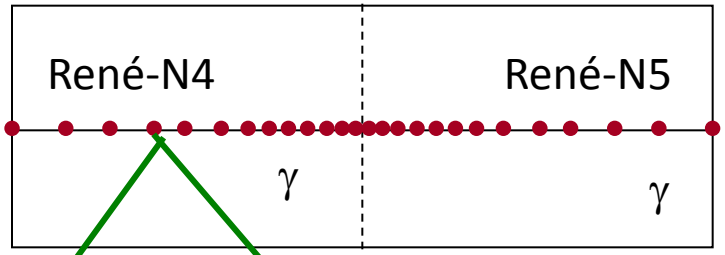
Auxiliary files (e.g. *.EXP)

- 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

CALPHAD Method for Multicomponent Diffusion

At each grid point for each time step for a given temperature profile.



LOTS of DATA need to be STORED!!!

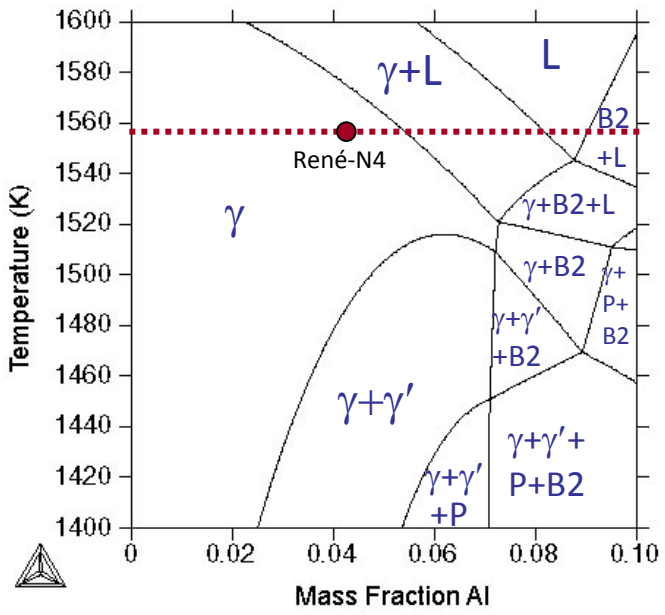
$$G^{\phi}(x,T,P) = G^{\circ} + G^{ideal} + G^{exess}$$

$$G^{n}_{jk} = M \cdot \nabla \mu$$

$$M^{\phi}_{i}(x,T,P) = M^{\circ} + M^{exess}$$

Thermodynamics

Diffusion matrix

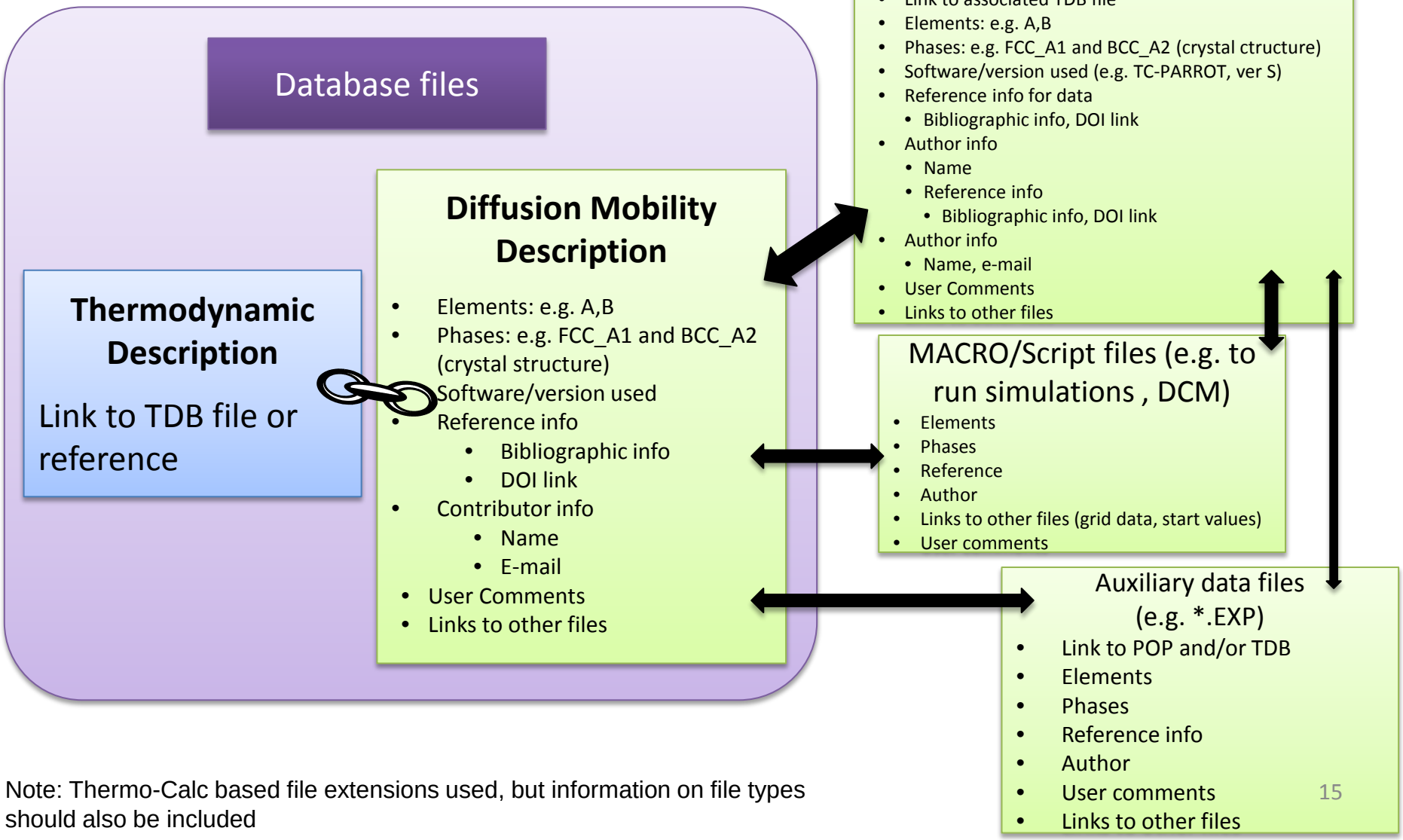


René-N4 ($x10^{-14}$ m^2/s) at 1293 °C

	Al	Co	Cr	Mn	Nb	Ta	Ti	W
Al	+119.5	+13.93	+34.83	+34.34	+42.43	+51.10	+49.51	+53.22
Co	-11.37	+17.00	-8.25	-5.67	-5.55	-1.83	-7.10	-9.69
Cr	-4.26	-5.37	+13.67	-3.21	+8.93	+9.91	+8.25	+2.49
Mn	-8.33	-0.280	-0.426	+7.57	-0.55	-0.36	-0.17	-0.45
Nb	+0.31	+0.25	+0.66	+0.27	+24.05	+0.74	+0.85	+0.31
Ta	-0.68	+0.33	+0.53	+0.24	+0.26	+0.76	+0.50	+0.23
Ti	+1.63	+1.35	+4.94	+4.94	+6.25	+6.57	+23.62	+5.41
W	-1.81	-0.62	-0.55	-0.60	-1.22	-0.83	-0.70	+3.40

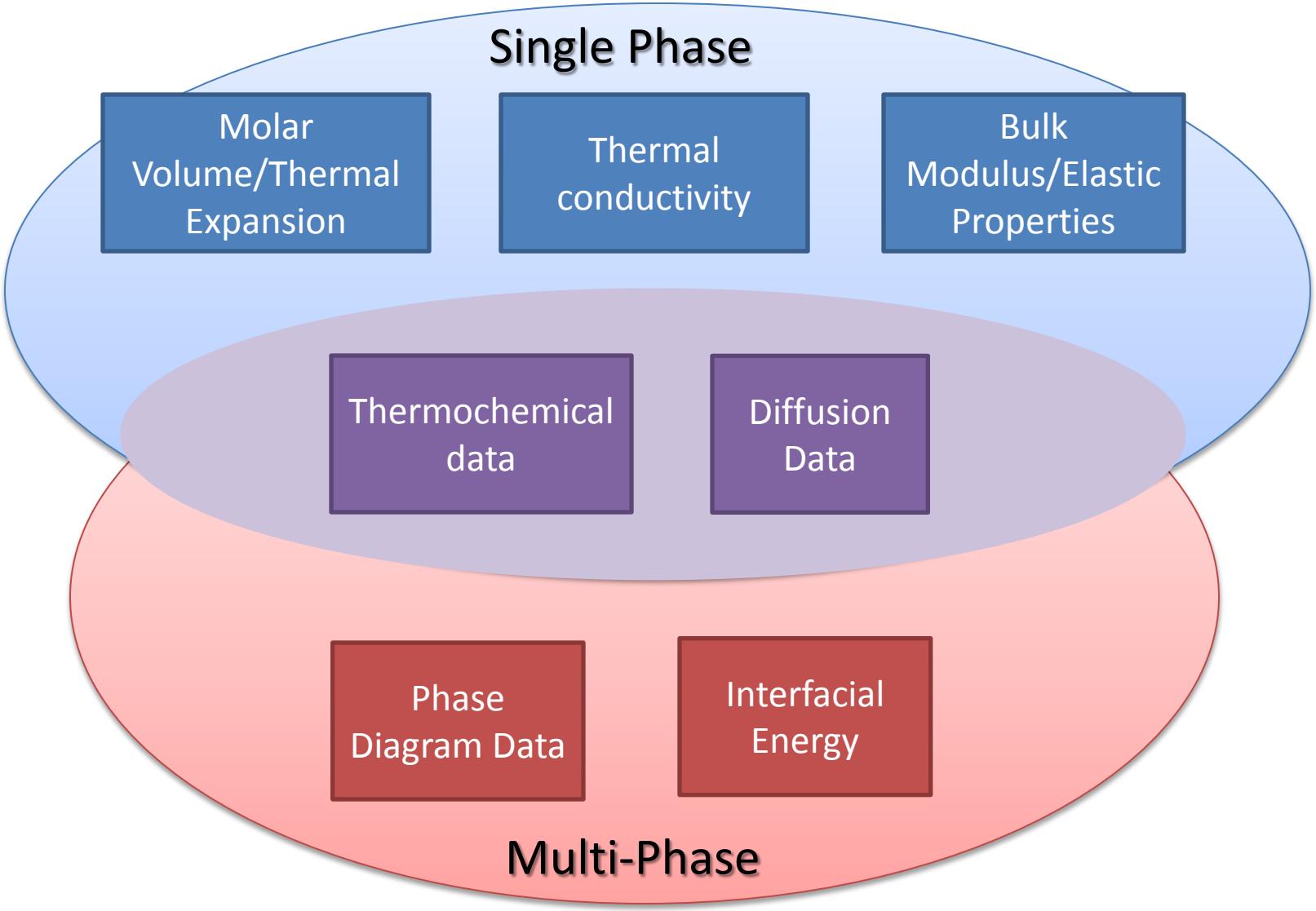
Efficient data storage and use

Examples of Files for a CALPHAD Diffusion Mobility Assessment



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

DATA (Experimental and Calculated)



Information Need to Describe a Data Entry

Data

- Elements present
- Type of value (e.g. enthalpy, heat of formation, phase boundary, diffusivity, lattice parameter, bulk moduli)
  - Experimental or computational method
  - Type of measurement (direct or indirect)
- Number of phases present
- Datum value and error
  - Type (single value or series)
  - Units
  - Actual value(s) and error(s)
- For each phase present
  - Phase name
  - Composition and fraction and errors
  - Crystal structure (this input will follow the format prescribed by the CCN) or amorphous
  - Lattice parameter
- Temperature and error
- Pressure and error

Metadata

- Type of material
  - Bulk composition
  - Material purity
  - Sample preparation
  - Microstructure information
    - Single crystal
    - Polycrystalline (grain size, dislocation density)
    - Non-crystalline
- Data manipulation details (if any, e.g. reference state corrections, analysis method to determine interdiffusion coefficient)
- Reporting format (raw data, digitized data, other)
- Reference (DOI or text ; one must be present)
- Additional information

Next Steps

- File repository for first principles calculations
- File repository for CALPHAD calculations
- General data repository
  - Prototype repository for data used in Calphad assessments
  - Evaluation of data storage formats (e.g. markup language, hierarchical data format)