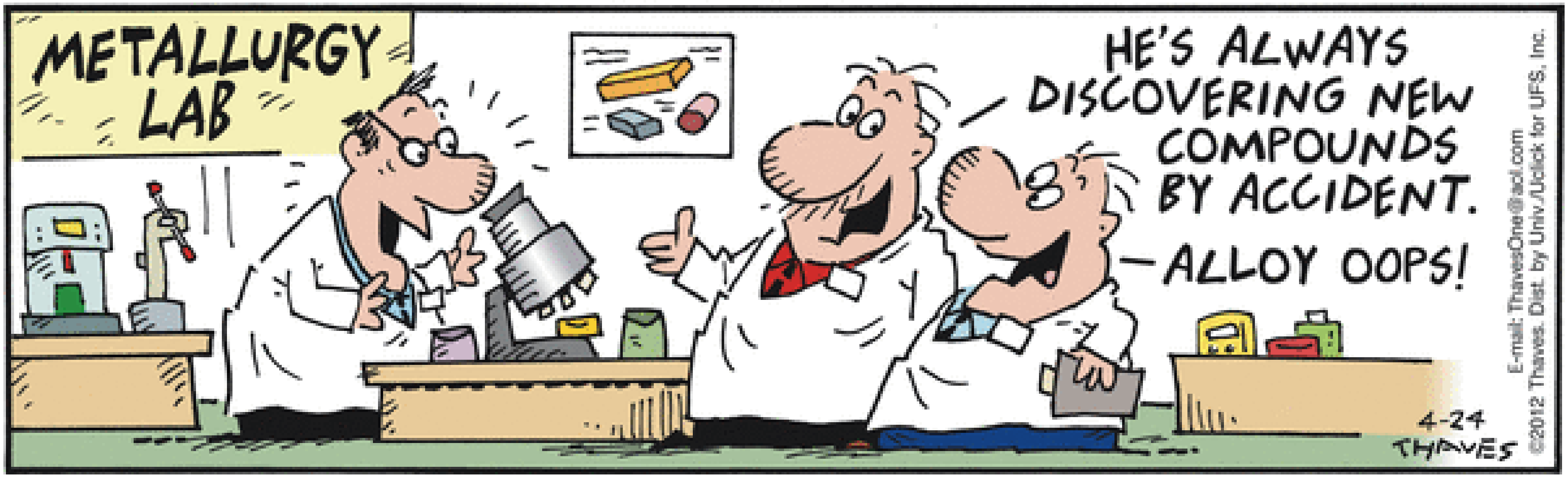
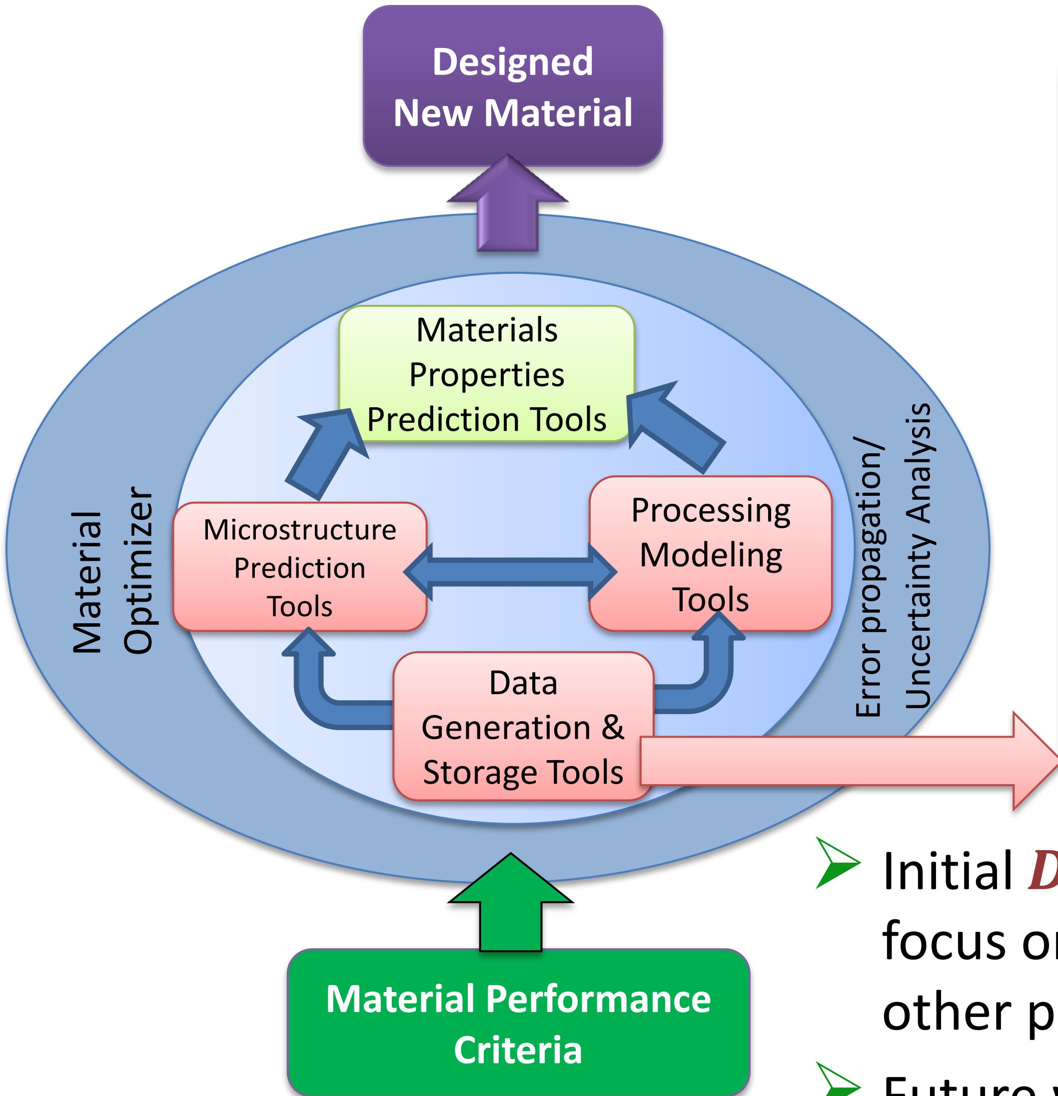



# MGI: Putting an End to Alloy Oops:* NEED DATA

**C. E. Campbell, U.R. Kattner, E. Lass,**
**Metallurgy Division, NIST**
**And**
**Laura Bartolo, Kent State University**

*Doug Foxvog, ITL

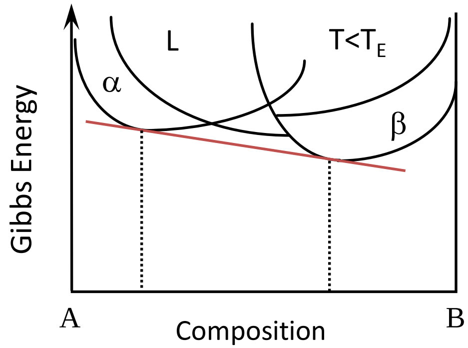
# Materials Data for the MGI

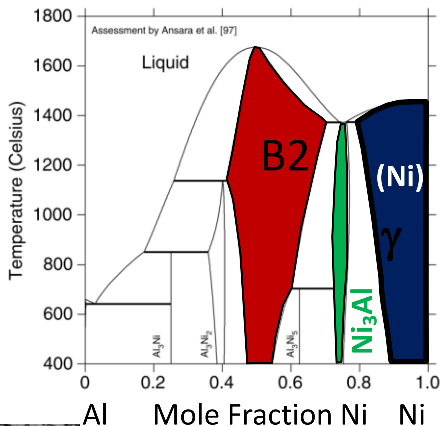


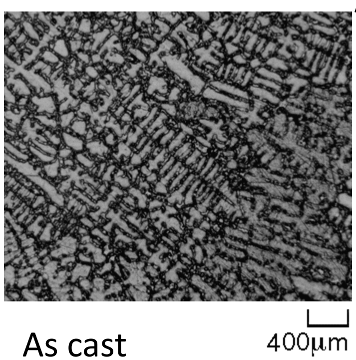

- Need to develop and curate materials information databases is well established.


- Initial ***Data &Tools*** development will focus on thermodynamics, kinetics and other phase-based material properties.
- Future work will build on this experience and expand into other areas.

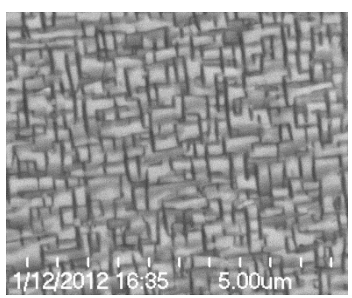
# Why Start with Thermodynamics, Kinetics and Phase-based Material Properties



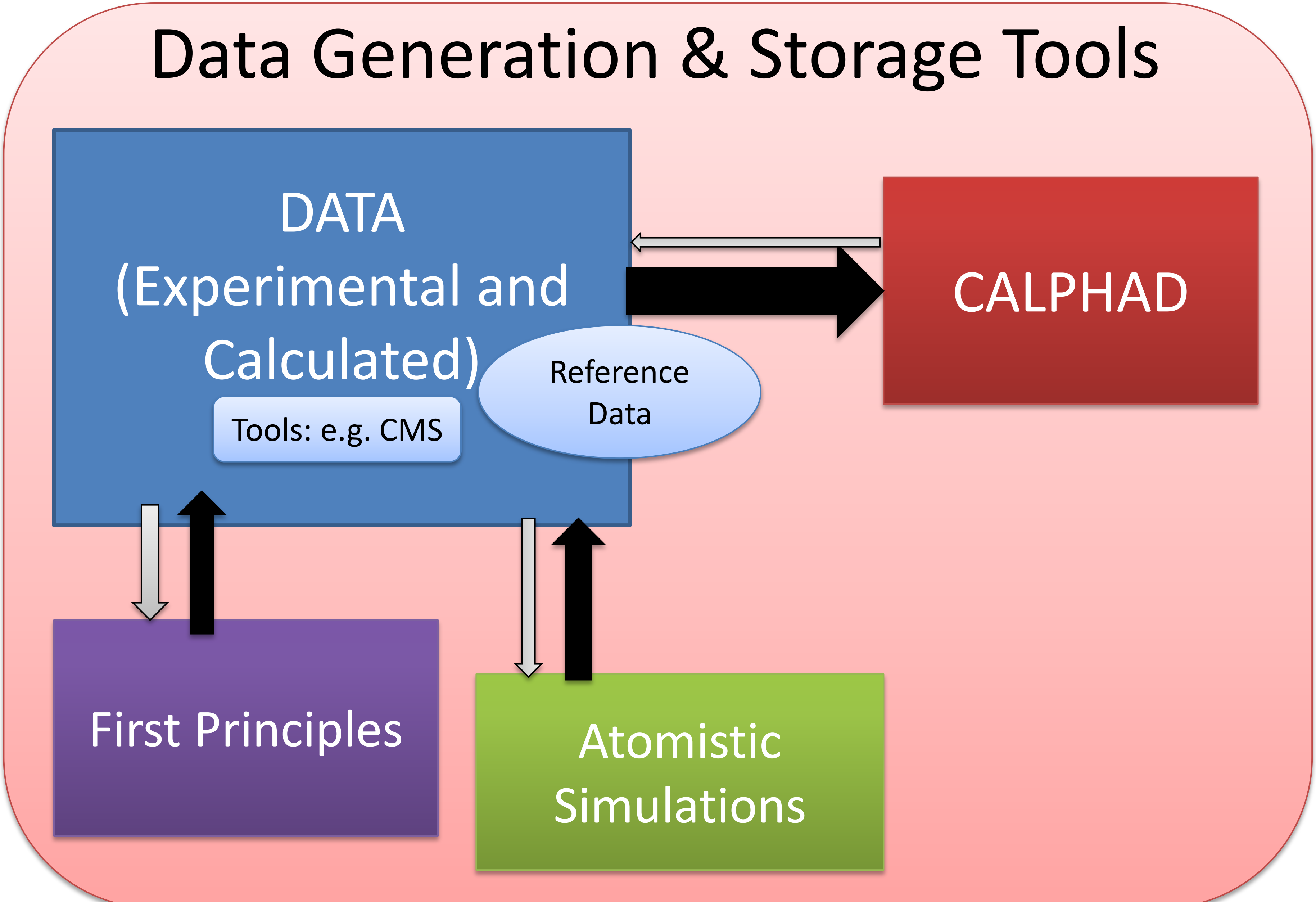




As cast microstructure

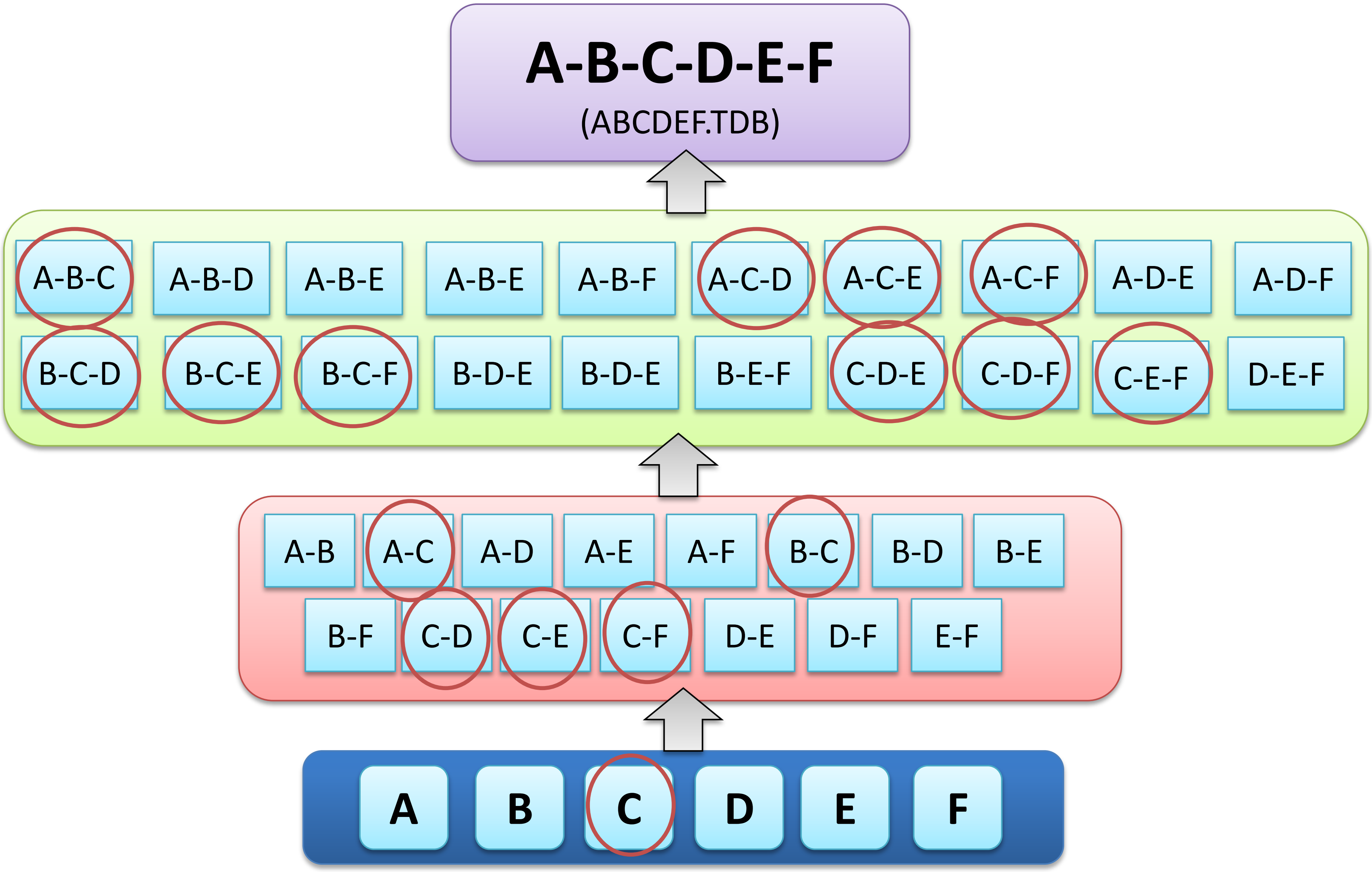



Annealed microstructure

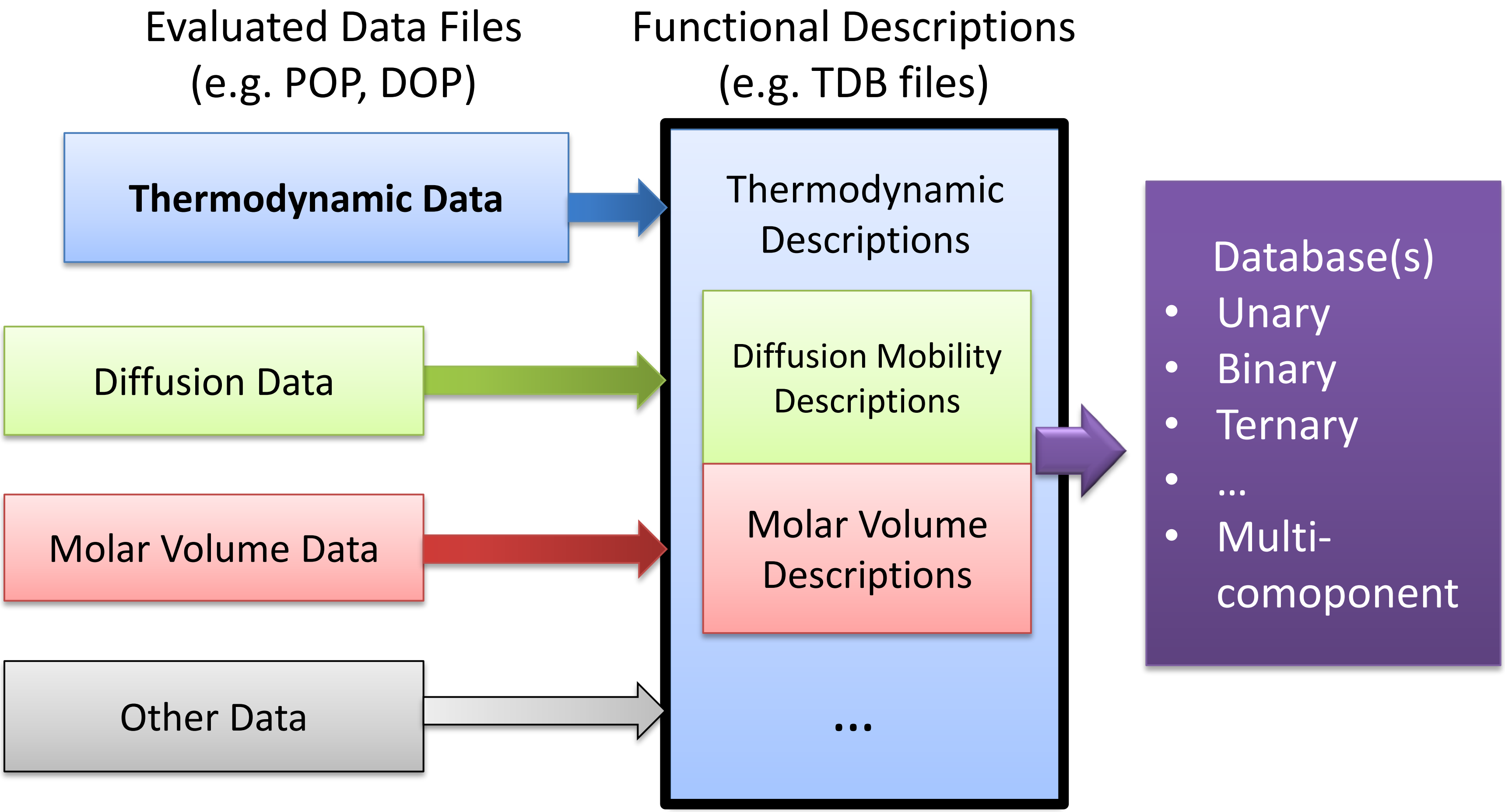
| | |
|---|---|
| Gibbs energy | $G = g(T, P, N_i)$ |
| Entropy | $S = -\left(\frac{\partial G}{\partial T}\right)_{P,N_i}$ |
| Enthalpy | $H = G - T\left(\frac{\partial G}{\partial T}\right)_{P,N_i}$ |
| Heat capacity | $C_P = -\left(\frac{\partial^2 G}{\partial T^2}\right)_{P,N_i}$ |
| Chemical potential | $\mu_i = \left(\frac{\partial G}{\partial N_i}\right)_{P,T,N_{j\neq i}}$ |
| 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 | ${}^{i}D_{jk} = N_j M_j \frac{\partial \mu_j}{\partial N_k}$ |


Data Generation & Storage Tools
DATA
(Experimental and
Calculated)
Tools: e.g. CMS
Reference
Data
CALPHAD
First Principles
Atomistic
Simulations

# Need for File Repository



# Structure of CALPHAD Database Files



# Examples of Files for a CALPHAD Diffusion Mobility Assessment

Linked to Searchable interface

## 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 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
- Author info
  - Name, e-mail
- User Comments
- Links to other files

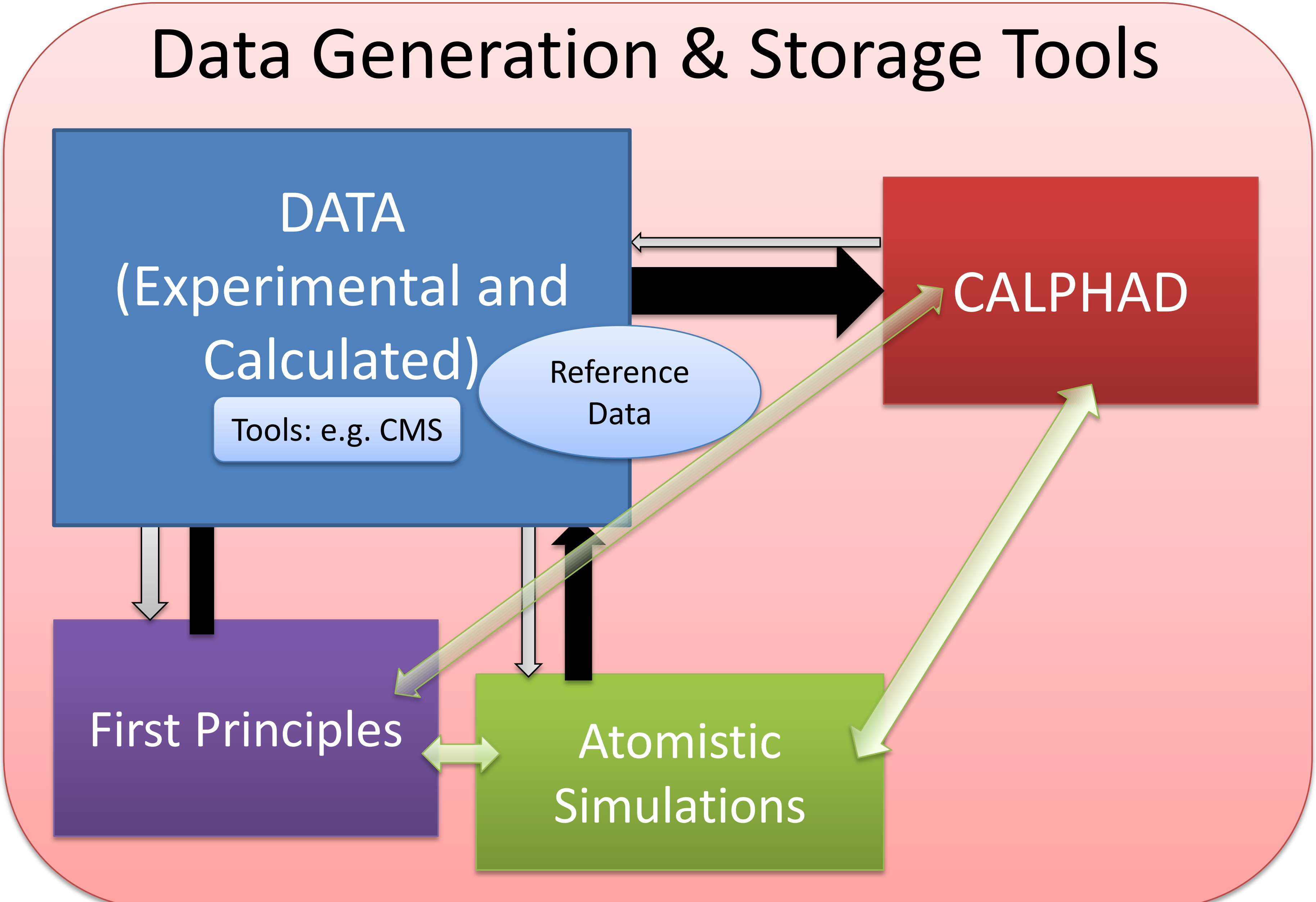
### MACRO/Script files (e.g. to run simulations , DCM)

- 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
- User comments
- Links to other files

Note: Thermo-Calc based file extensions used, but information on file types should also be included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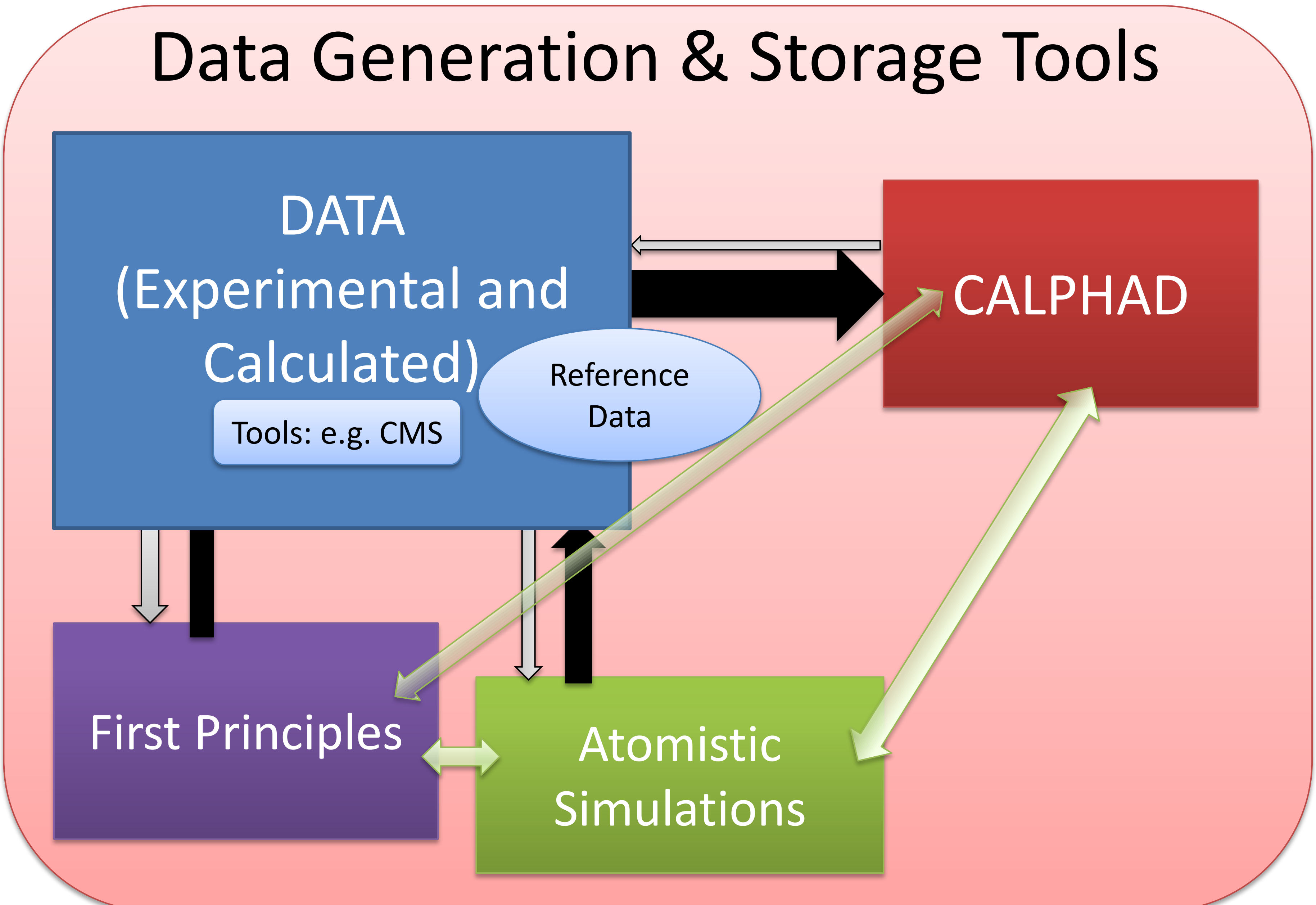
Tools: e.g. CMS
Reference Data
CALPHAD
First Principles
Atomistic Simulations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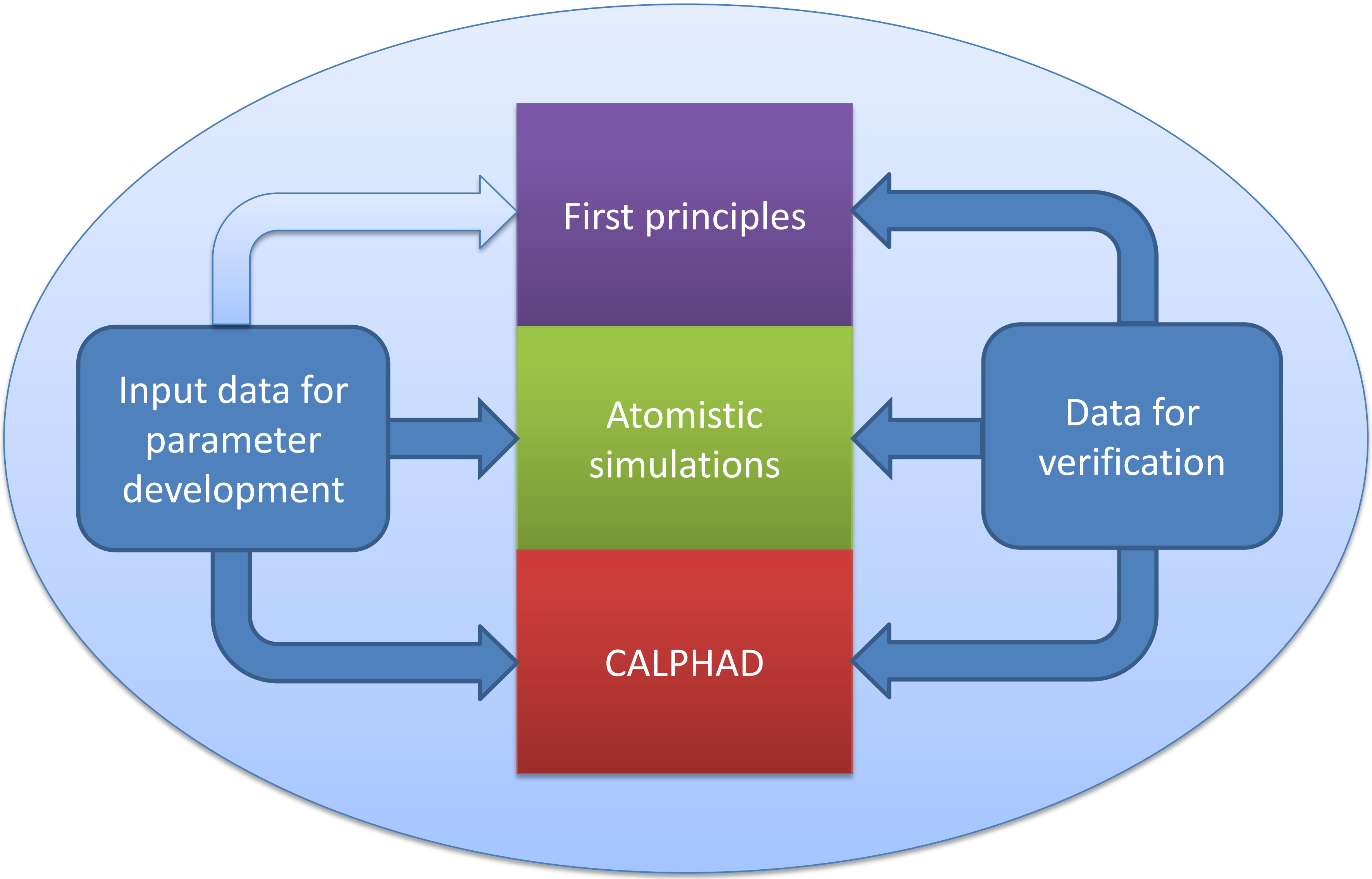
# Computational Methods and Data



# Information Need to Describe General 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 CC[illegible]) or amorphous
    - Lattice parameter
- Temperature and error
- Pressure and error

## Metadata

- Type of material
    - Bulk composition
    - Material purity
    - Sample prepa
    - Microstructur
        - Single c
        - 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

**Need flexible formats that can evolve with changing data needs!**

# Identifiers

- **Crystal Structure**
  - Materials consist of distinct phases which are characterized by their crystal structures.
  - Crystallographic data *(lattice parameter(s), space group symmetry, positional parameters)* for a phase convey the identities of constituent atoms as well as their exact positions in space.
  - Information on the identities and arrangement of constituent atoms (crystallographic data) provide the initial critical input for modeling materials behavior.
  - ➢ Use the InChI identifier (Space group & wycoft sites)

- Material (Composition, Heat Treatment, + ???
  - InChI type identifier

# Diffusion Data Types

- Tracer Diffusivity
- Intrinsic Diffusivity
- Interdiffusion
- Grain boundary diffusion
- Activation Energies
- Diffusion Couple Composition Profiles
- Layer widths

Could be reported as a function or individual determined diffusivites .

Need to know temperature, composition, phases, present, and diffusing species

## Metadata Need:

- 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

# Things to Consider

- Naming conventions for files
  - ABC_Smith05.xxx
- Files to reproduce a specific DICTRA simulation store together in a zip or separate linked files in workspace

# Concepts for Workspace/Workflow

- An individuals can have multiple different workspaces.
  - AlCu-Thermodynamics;  CoNi-Diffusion,  ReNi-Experimental. AlTi-FirstPrinciples

- Owner of the workspace defines who has access to the workspace and what the level of access is.

- Workspaces can be shared between different groups/worskspaces

- Workspaces would have some basic structure elements specific to the type of workspace.
  - Thermodynamics, Diffusion,  Experiments  (types of workspace)
  - Common structural elements: People, Types of Resources, Systems

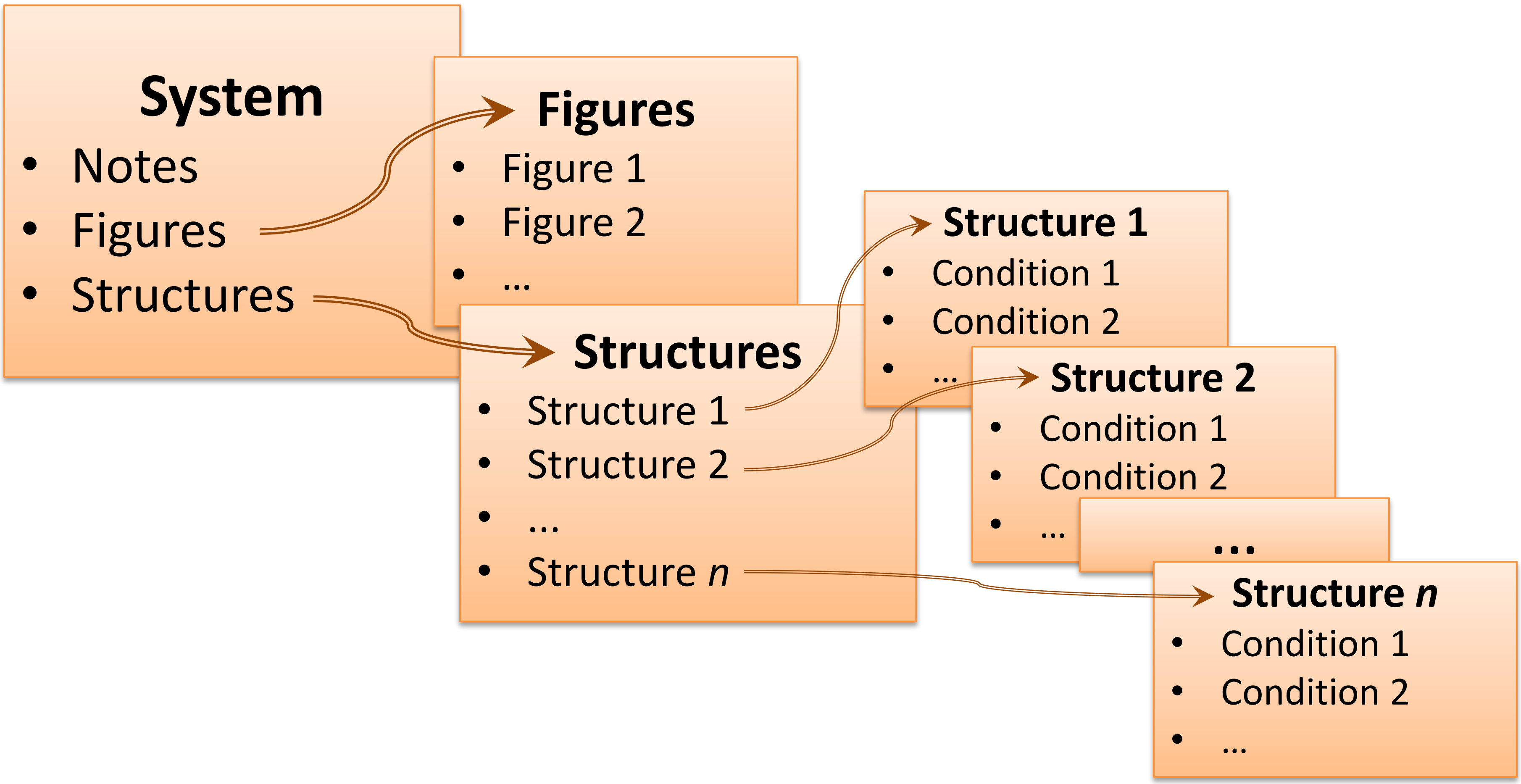
# Discussion Points – What's workable?

- - Naming conventions for files & workspaces
- - Files to reproduce a specific DICTRA
- - Some files stored in zip; others as separate linked files
- - Start with 8 categories:
  - People; Phased Based Materials Properties; Phases; Software; Systems; Techniques; Treatments; Types of Resources

# File Repository for ATAT-MAPS Data Structure

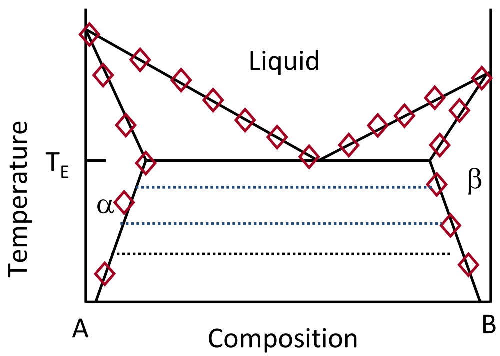
## Chemical Systems:

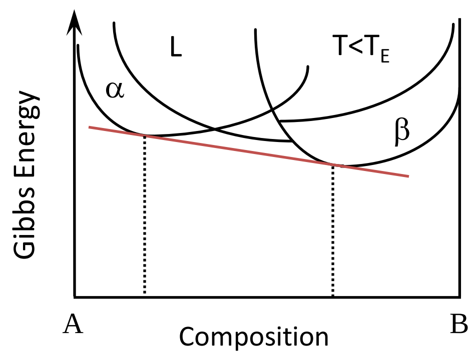
Au-Cu, NaCl-KCL, SiC-AlN, AlN-GaN-InN, …

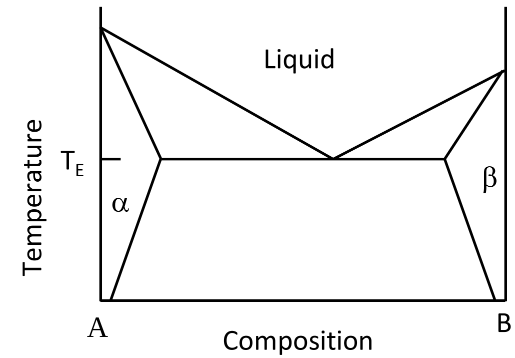


# Original CALPHAD Approach

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 methodology can be applied to the description of other property data**