# OpenCalphad - Open Source Thermodynamic Software

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## Motivation

Thermodynamic data are essential for the understanding, developing, and processing of materials. The CALPHAD (Calculation of Phase Diagrams) technique has made it possible to calculate properties of multicomponent systems using databases of thermodynamic descriptions with models that were assessed from experimental data. A number of CALPHAD software are available for the calculation of properties of multicomponent systems, and the majority are commercial products. However, the use of thermodynamics in many applications suffers from the lack of availability of free high quality software for multicomponent systems. The aim of the OpenCalphad (OC) software is to fill this gap.
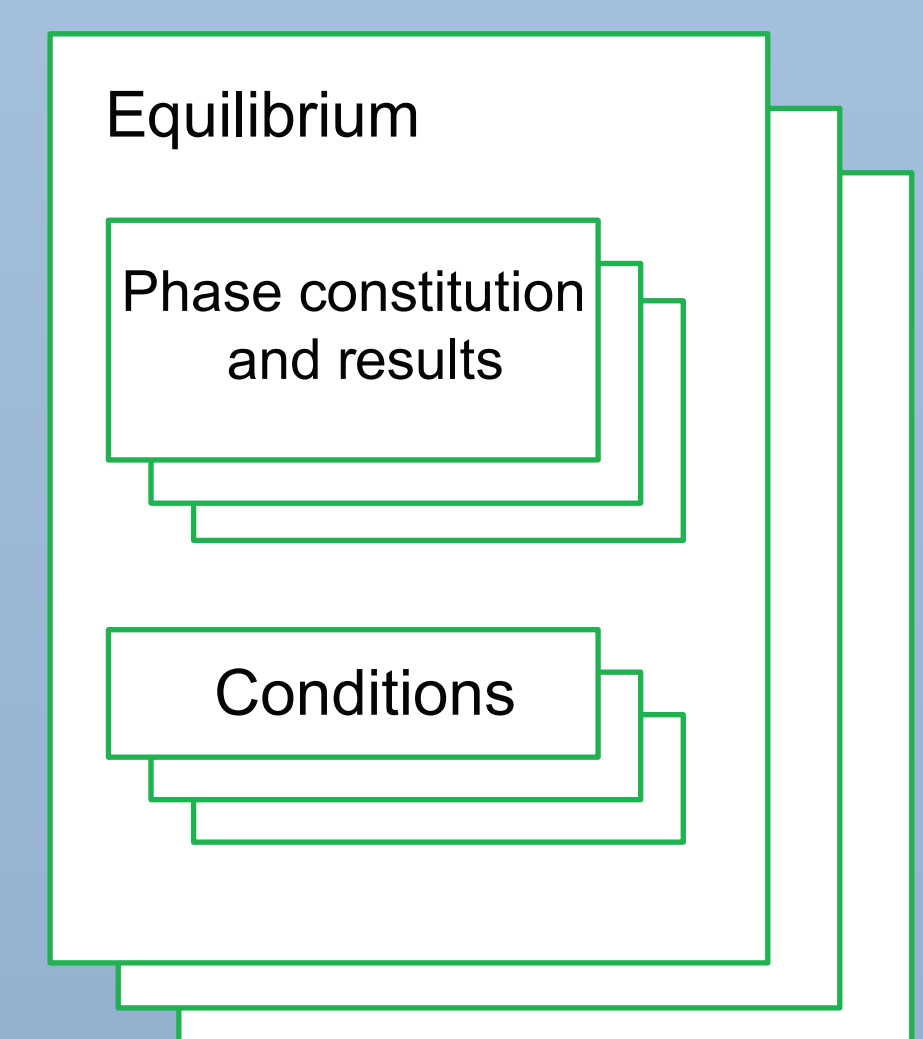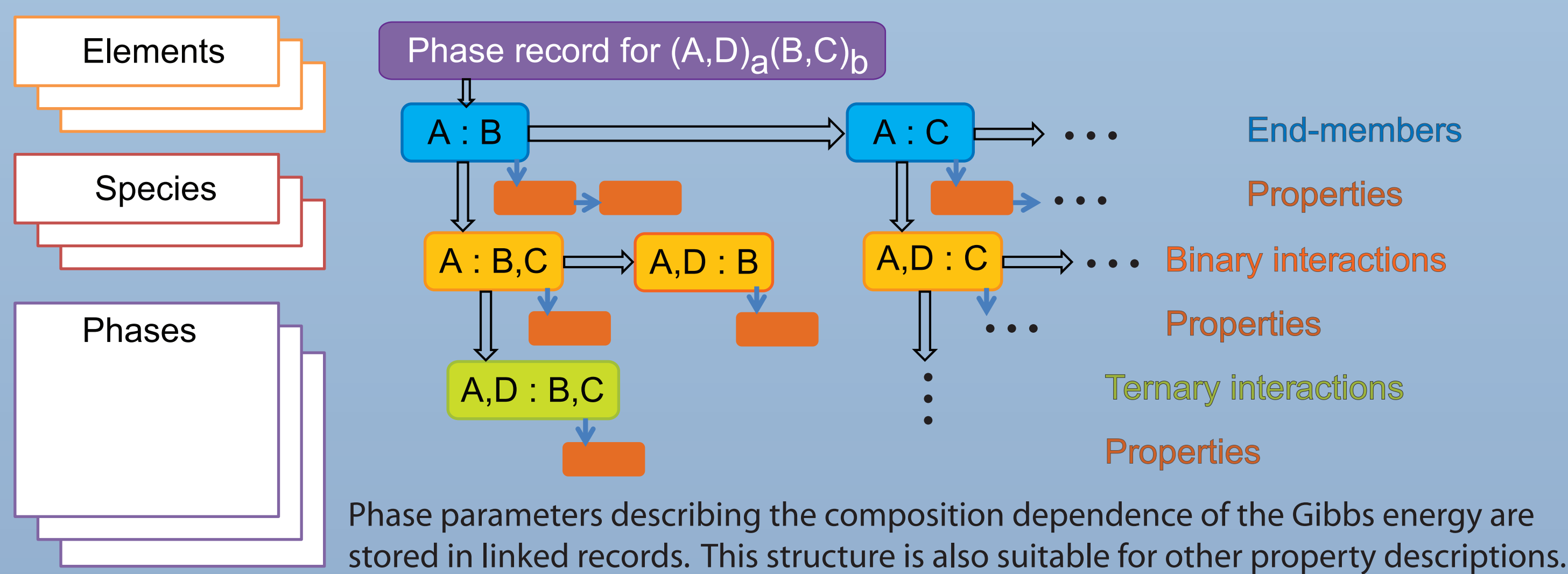
The OC software has a simple programming interface to facilitate integration in application software. This is important for coupling validated thermodynamic as well as kinetic data in process simulations or using the results of thermodynamic calculation in high-throughput alloy selection. Such use of thermodynamic calculations requires that a number of results needs to be obtained within reasonably short time, making the abilty of parallel processing highly desirable. At present, no other high quality open source software is available for calculations of multicomponent systems using CALPHAD-type models or allows these calculations using parallel processing.

## Data structures

The organization of the variable space into static and dynamic records in OC is essential for efficient parallel processing.

The thermodynamic description of system is static in OC memory as it does not change with the external conditions.

External conditions and calculated results are stored in dynamic records.



Phase parameters describing the composition dependence of the Gibbs energy are stored in linked records. This structure is also suitable for other property descriptions.

## Gibbs energy minimization

A Lagrange function is constructed taking into account external conditions and internal contraints using Lagrange multipliers.

$$ L = G + \sum_A \left( N_A - \sum_\alpha \aleph^\alpha M_A^\alpha \right) \mu_A + \sum_\alpha \sum_s \eta^{\alpha,(s)} \left( \sum_i y_i^{\alpha,(s)} - 1 \right) $$

G is the Gibbs energy of the system, $\aleph^\alpha$ is the amount of formula units, $N_A$ is the total amount of component A, $M_A^\alpha$ is the amount of A in phase $\alpha$, $s$ is the sublattice index, and $y_i^{\alpha,(s)}$ is the constituent fraction of species, $\mu_A$ and $\eta^{\alpha,(s)}$ are the Lagrange multipliers.

A Grid minimizer ensures determination of the true equilibrium instead of a metastable one.
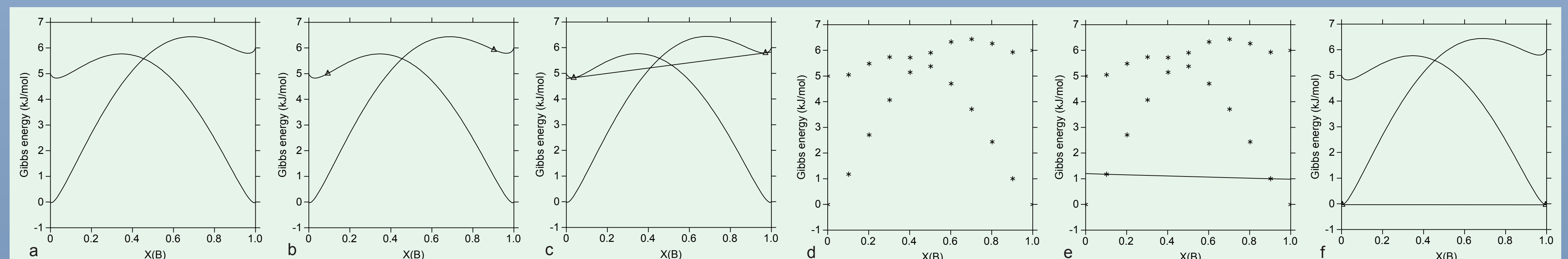


With the given Gibbs energy cures (a) the use of estimated start values (b) my result in finding a metastable equilibrium (c) while the grid minimizer calculates a number of points along the Gibbs energy cuves (d) using the compositions with the lowest Gibbs energies (e) as start values to find the true equilibrium (f).

## Graphical display of results
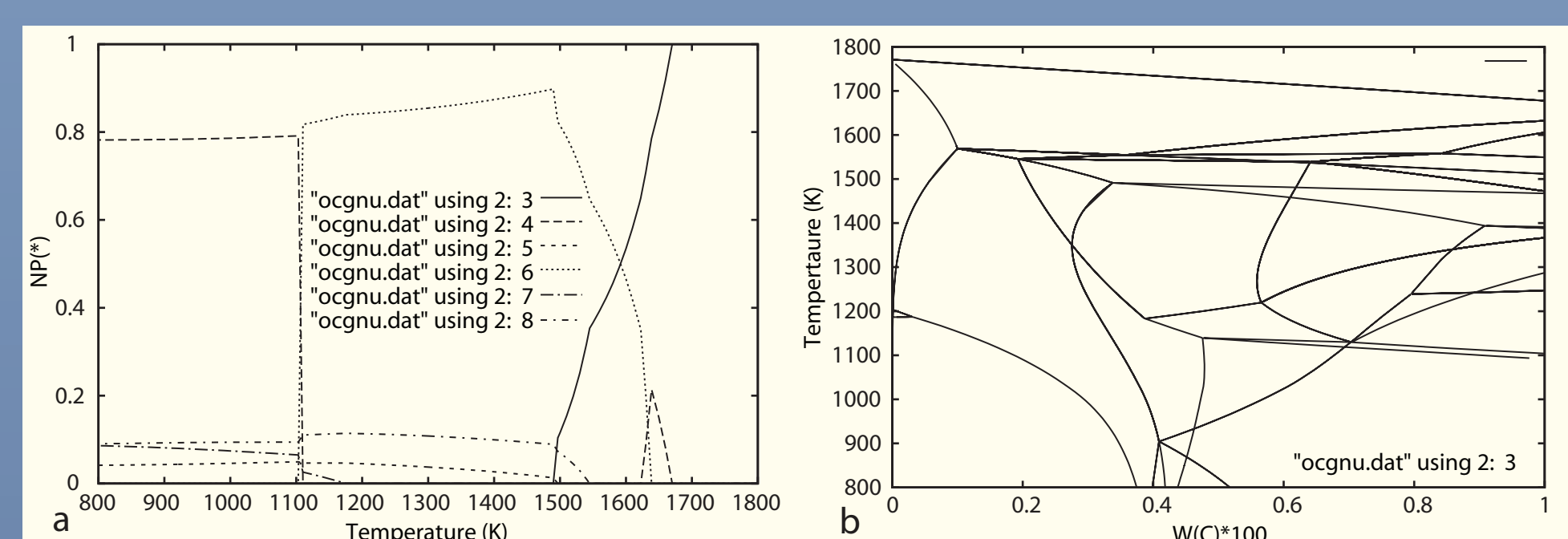


Results from stepping and mapping calculations of a six-component high speed steel at varying temperatures plotted with Gnuplot, the phase amounts (a) and the phase diagram (b).

## Software library for application programs

Examples of interface functionality

| Routine | Action |
| --- | --- |
| read_data | Read materials data for a selected set of elements and phases from the database file |
| set_condition | Set a condition for T, P, composition, chemical potential, stable phase, etc. Each condition can be set and changed separately. Simulations can use multiple equilibria with different conditions to represent local equilibrium. |
| calculate_equilibrium | Calculate the equilibrium for the given set of conditions. |
| get_value | Obtain the calculated value of a chemical potential, amount, or composition of a phase, atomic mobility of a component, etc. |

The availability of open source code will greatly benefit scientists in academia as well as in industry in the development of new models and assessment of model parameters from both experimental data and data from first principles calculations and explore direct coupling of thermodynamic calcuclations in a variety of simulations.