

The OpenCalphad software, a status report 2018

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Objective

The OpenCalphad (OC) is an informal collaboration between scientists interested in developing a free high quality thermodynamic software. At present OC provides:

- ▶ a platform to implement new thermodynamic models,
- ▶ a fast and reliable algorithm for equilibrium calculations,
- ▶ facilities to calculate property and phase diagrams,
- ▶ possibilities to assess model parameters and develop assessment techniques,
- ▶ a software interface for integration in materials simulation programs.

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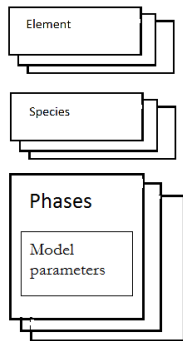
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- ▶ a software interface for integration in materials simulation programs.

Additionally OC can calculate equilibria in parallel.

Current release from 2017 at <http://www.opencalphad.org>

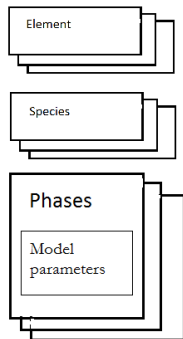
A new release will be available shortly when the documentation of the development version at <http://github.com/sundmanbo/opencalphad> has been finished.

Static and dynamic data



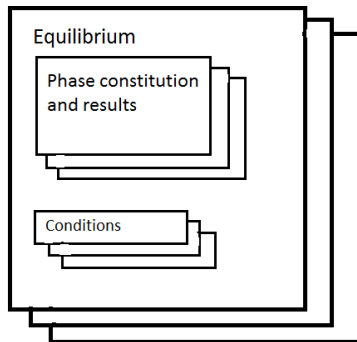
The data for elements, species and model parameters are independent on the external conditions on the system and makes up the “static” data.

Static and dynamic data



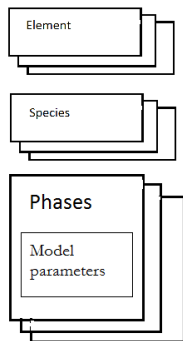
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Dynamic data



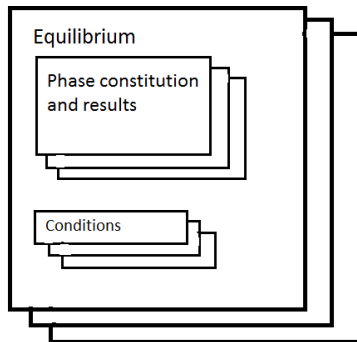
The external conditions and calculated results for the amount and constitution of the phases is the dynamic data and is stored in an equilibrium record.

Static and dynamic data



The data for elements, species and model parameters are independent on the external conditions on the system and makes up the “static” data.

Dynamic data



In the dynamic data structure each equilibrium record is has a separate set of conditions and results and they can be calculated in parallel.

Bottom up data



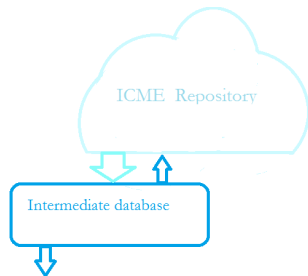
Thermodynamic databases grow from the bottom

Top down use

The materials genome and ICME initiatives will create large materials data repositories. Most likely several separate dataset will be stored for many systems and for an application a selection must be made and stored in intermediate database files.

A TDB file is one kind of such databases for use in thermodynamic calculations and simulations.

The TDB format was a proposal from SGTE more than 30 years ago to provide a standard of data transfer between different software.



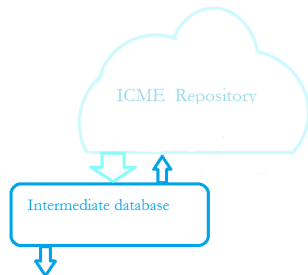
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A generalized “Portable materials property Data Base” (PDB) format has been proposed as an update of the TDB format.



Parameter property identifier

An property of great interest for materials simulation is the mobility of a component A in a phase. Inside OC there are many property identifiers which can depend on T, P and constitution of the phases.

Indx	Ident	T	P	Specification	Status	Note
1	G	T	P		0	Energy
4	CTA	-	P		2	Curie temperature
5	NTA	-	P		2	Neel temperature
6	IBM	-	P	&<constituent#sublattice>;	12	Individual Bohr magneton num
7	THET	-	P		2	Debye or Einstein temp
8	MQ	T	P	&<constituent#sublattice>;	10	LN mobility1 of component
13	G2	T	P		0	Liquid two state parameter
14	VISC	T	P		0	Viscosity
15	LPX	T	P		0	Lattice param X axis
16	LPY	T	P		0	Lattice param Y axis
17	LPZ	T	P		0	Lattice param Z axis
19	EC11	T	P		0	Elastic const C11
20	EC12	T	P		0	Elastic const C12
21	EC44	T	P		0	Elastic const C44
23	VO	-	-		1	Volume at T0, P0
24	VA	T	-		4	Thermal expansion
26	LAMB	T	P		0	Thermal conductivity

During an equilibrium calculation these property parameters can be calculated for the current T, P and composition of the phases at the same time as the Gibbs energy.

Calculating the equilibrium state

The equilibrium at fixed temperature, pressure and composition is given by a minimum in the total Gibbs energy of the system. The thermodynamic models describe the molar Gibbs energy, G_M^α and the total energy for the system is:

$$G = \sum_{\alpha} N^{\alpha} G_M^{\alpha} \quad (1)$$

where N^{α} is the amount of the stable phases.

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The algorithm used in OC was published by Mats Hillert in 1981 and its implementation on OC in 2015.

It is a much more flexible and faster method for equilibrium calculations than using any kind of “common tangent” construction.

Global grid minimizer provides start values

Hillert's algorithm is iterative and depends strongly on the initial set of stable phases and their constitutions.

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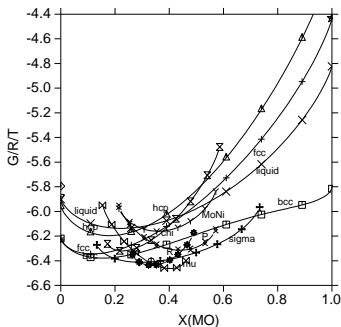
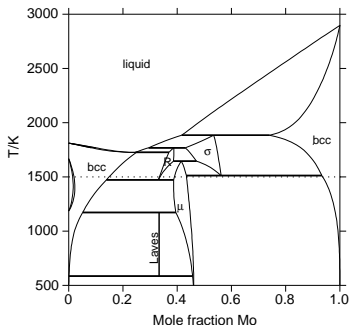
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The grid minimizer will also automatically find miscibility gaps.

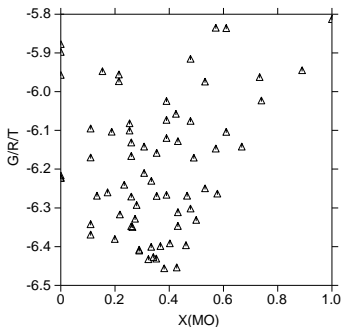
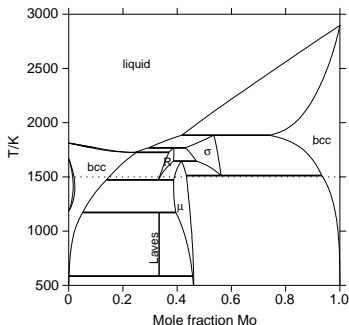
Grid minimizer, an example

In the Fe-Mo system at 1500 K the grid minimizer calculates a number of points along the Gibbs energy curves of the different phases.



Grid minimizer, an example

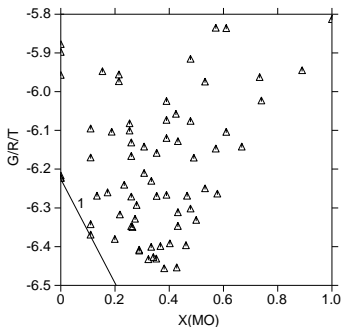
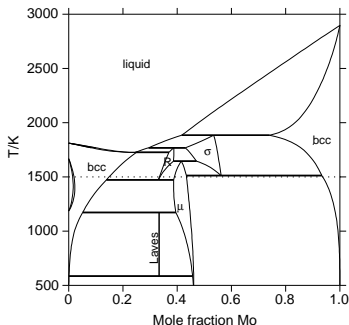
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The gridpoints are treated as individual stoichiometric phases by the grid minimizer.

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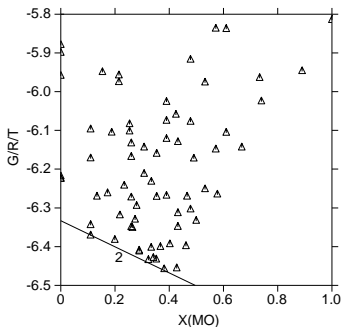
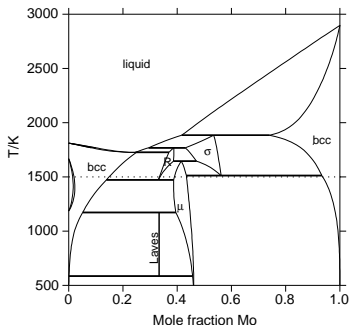
In the Fe-Mo system at 1500 K the grid minimizer calculates a number of points along the Gibbs energy curves of the different phases.



For low Mo content these two gridpoints will be selected as starting constitutions. They represent the FCC and BCC solution phases.

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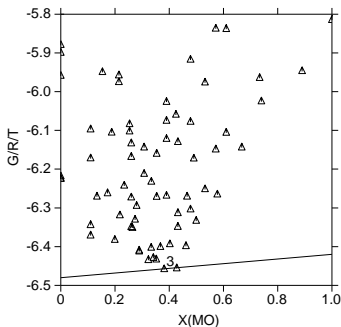
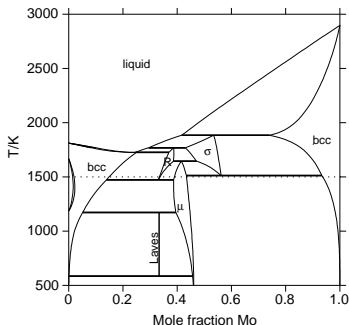
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For higher Mo content these two gridpoints will be selected. They represent the BCC and μ phases. The iterative algorithm when then replace either BCC or μ with the R phase.

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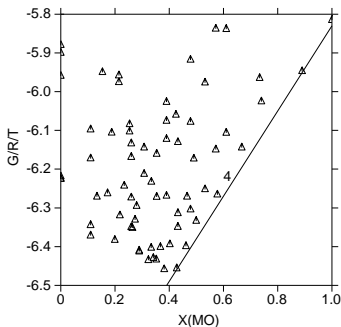
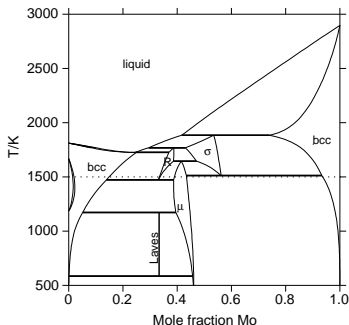
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For Mo content around 40% these two gripoints will be selected. They are both in the μ phase and the iterative algorithm will merge them into a single composition.

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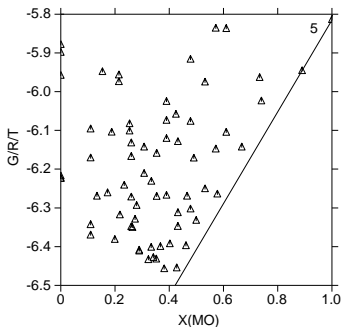
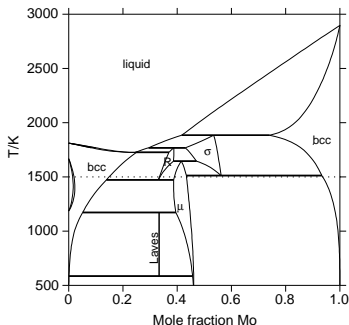
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At higher Mo content one gridpoint in the μ and another in the Mo-rich BCC phase will be selected.

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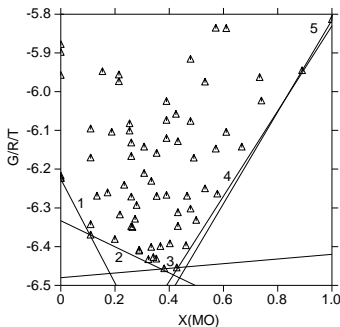
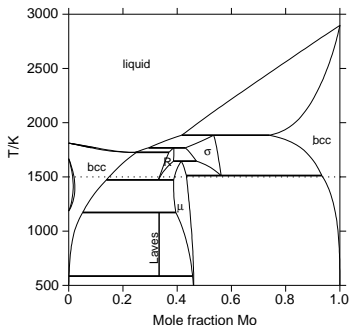
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For very high Mo content these two gridpoints in the BCC phase will be used as start points. They will merge to a single composition during the iterative minimization.

Grid minimizer, an example

In the Fe-Mo system at 1500 K the grid minimizer calculates a number of points along the Gibbs energy curves of the different phases.



Here is the convex hull represented by the gridpoints.

The density of the grid can be selected but more gridpoints require longer computational times. When calculating diagrams OC uses the previous calculated equilibrium as startpoint but occasionally global tests can be made.

STEP, MAP and PLOT procedures

The command STEP will calculate equilibria at fixed values along a single axis and additionally the exact axis value when the set of stable phases changes. Many different state variables can be plotted as a function of this axis variable from one step calculation.

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When the set of stable phases changes one has a “node point” where several lines meet and start points for these are generated.

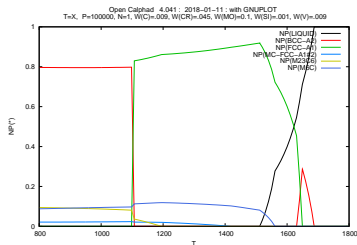
STEP, MAP and PLOT routines

The PLOT command creates a file for the GNUPLOT software with two axis variables specified by the user. This file can be further manipulated within the GNUPLOT software.

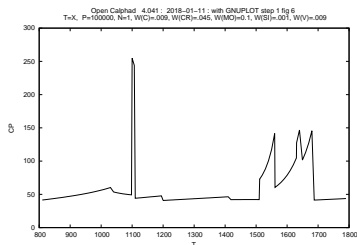
STEP, MAP and PLOT routines

Some examples of diagrams generated by OC. Macro files to generate these are provided with the software.

A phase fraction plot of a 6 component High Speed Steel (HSS)



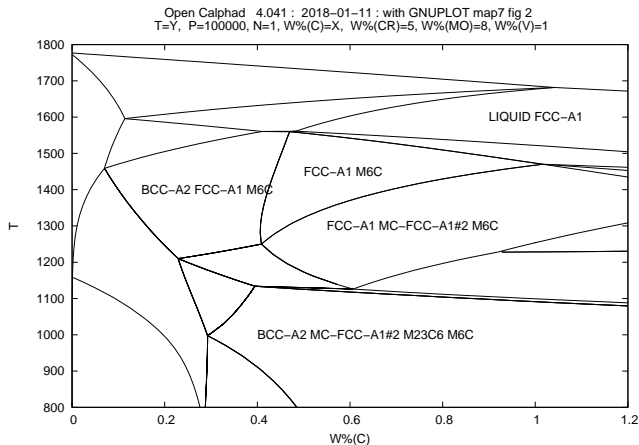
and from the same calculation we obtain how the heat capacity varies with T .



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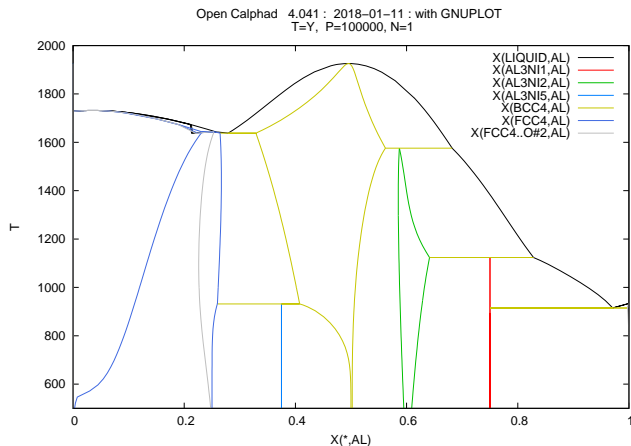
An isoploeth for the same HSS steel



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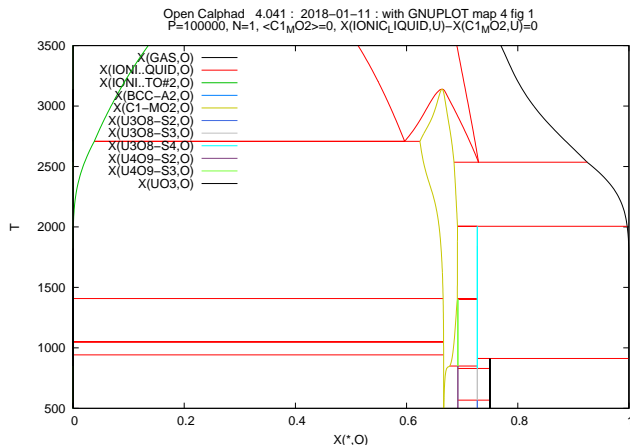
The Al-Ni phase diagram



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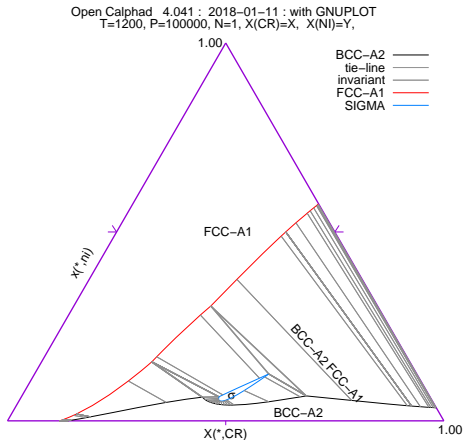
The O-U phase diagram



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An isothermal section at 1200 K for Cr-Fe-Ni



OC Application Software Interface, OCASI

OCASI is based on the TQ standard for thermodynamic software interfaces, used by Thermo-Calc and ChemApp, and provides similar facilities.

An advantage is that OCASI is available as source code so it can be modified by the application programmer and compiled on different hardwares, OS or compilers.

Example, solidification and homogenization

An aluminum company in France has converted a software they used for simulating solidification and homogenization to use OCASl.

They used an alloy with the composition

Si	Fe	Cu	Mn	Mg	Zn	Ti	Zr	Al
0.06	0.06	1.8	0.1	2.3	8.1	0.06	0.06	rest

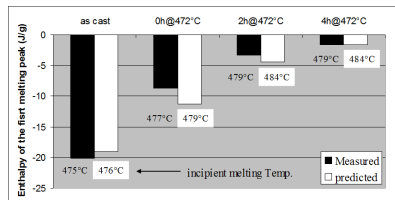
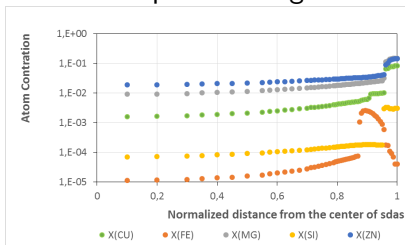
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Their own software took about 3.5 days to simulate the solidification and several subsequent homogenization steps.



The left hand figure show the concentration profiles across a dendrite after solidification, the right the heat evolved during homogenization.

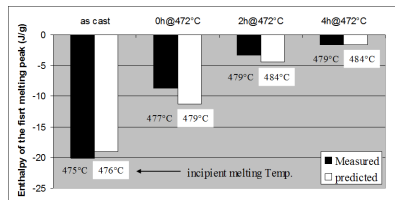
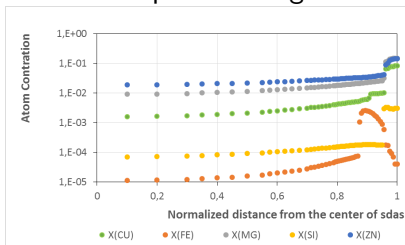
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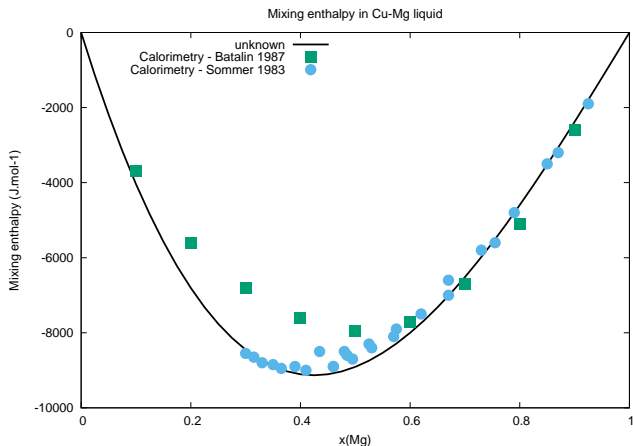
After implementing OCASI the same simulation took 3.5 hours using 12 CPUs in parallel, a gain of time with a factor of 24.

Assessment

A routine developed in Argonne National Lab for least square fitting has been included to minimize differences between experimental data and the same data calculated from the models by varying selected model parameters.

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The calculated enthalpy of mixing in the liquid Cu-Mg system overlayed with experimental data.

Current development status

What is working:

- ▶ Compound Energy Formalism (CEF) and ionic liquid models
- ▶ Magnetic and order/disorder models
- ▶ Reading (unencrypted) TDB files and entering data interactively
- ▶ Command oriented user interface with macro facilities
- ▶ Setting many different types of conditions, also relations between state variables
- ▶ Calculating multicomponent equilibria
- ▶ STEP calculation of property diagram
- ▶ MAP of binary, ternary and multicomponent phase diagram
- ▶ PLOT using GNUPLOT software
- ▶ The software interface, OCASI, is stable and flexible
- ▶ OC/OCASI can calculate many multicomponent equilibria in parallel
- ▶ Assessment of model parameters

Current development status

What is still in the pipeline:

- ▶ More models in particular for unaries and short range ordering.
- ▶ A new PhD student will develop the assessment module.
- ▶ Improving convergence and stability of calculations
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The best of all: The code is free so anyone interested can participate.

Download and references

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- ▶ Bo Sundman, Ursula R Kattner, Mauro Palumbo and Suzana G Fries, *OpenCalphad - a free thermodynamic software*, Integr Materials and Manufact Innovation, **4**:1 (2015)
- ▶ Bo Sundman, Xiao-Gang Lu and Hiroshi Ohtani, *The implementation of an algorithm to calculate thermodynamic equilibria for multi-component systems with non-ideal phases in a free software*, in Comp Mat Sci, **101** (2015) 127-137
- ▶ Bo Sundman, Ursula R Kattner, Christophe Sigli, Matthias Stratmann, Romain Le Tellier, Mauro Palumbo, Suzana G Fries; *The OpenCalphad thermodynamic software interface*, Comp Mat Sci **125** (2016) 188-196