The Application Software Interface for the Open Calphad software with some examples

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Background

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In this presentation I will provide an short description of the OC Application Software Interface (OCASI) and some examples how this can be used.
In addition to be free OC can also be run in parallel using the OpenMP library which can reduce the calculation times for a simulation more than one order of magnitude.

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- Summary and availability

Thermodynamic data

In the Calphad technique the Gibbs energy for each phase is modeled as a function of T, P and its constitution.

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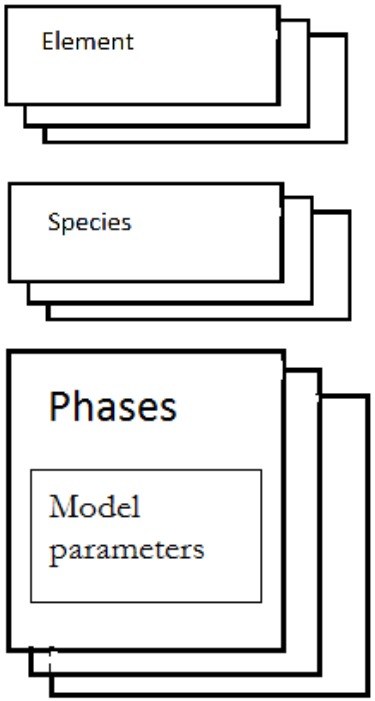
Static and dynamic memory



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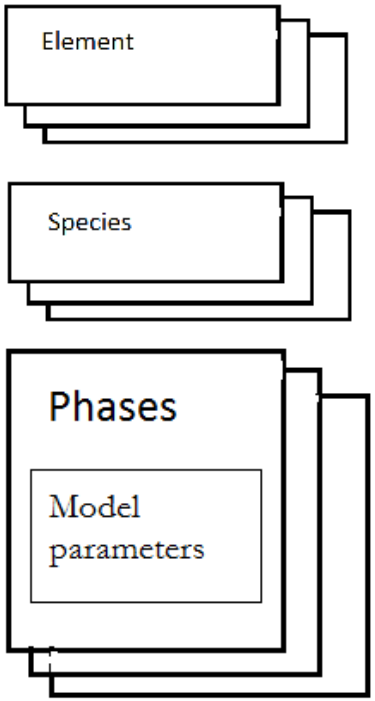

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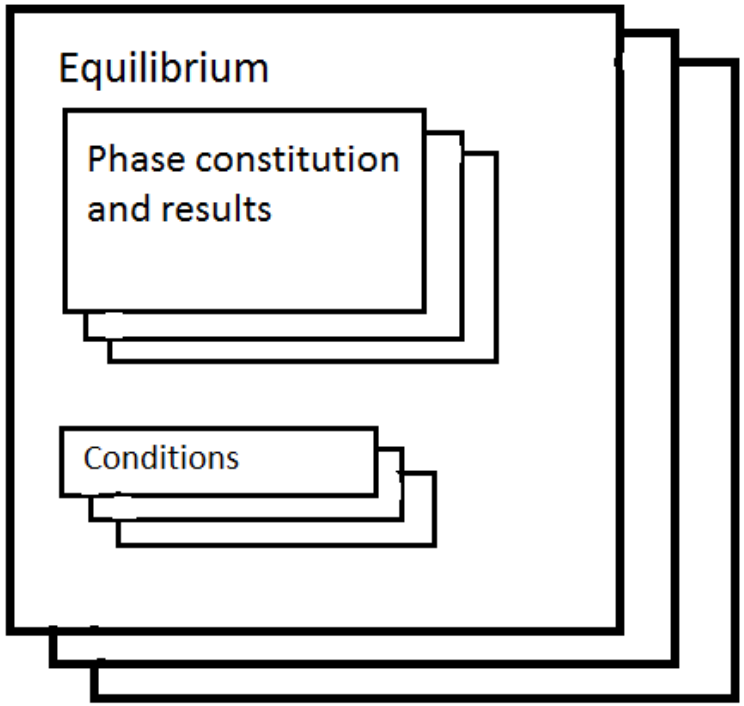
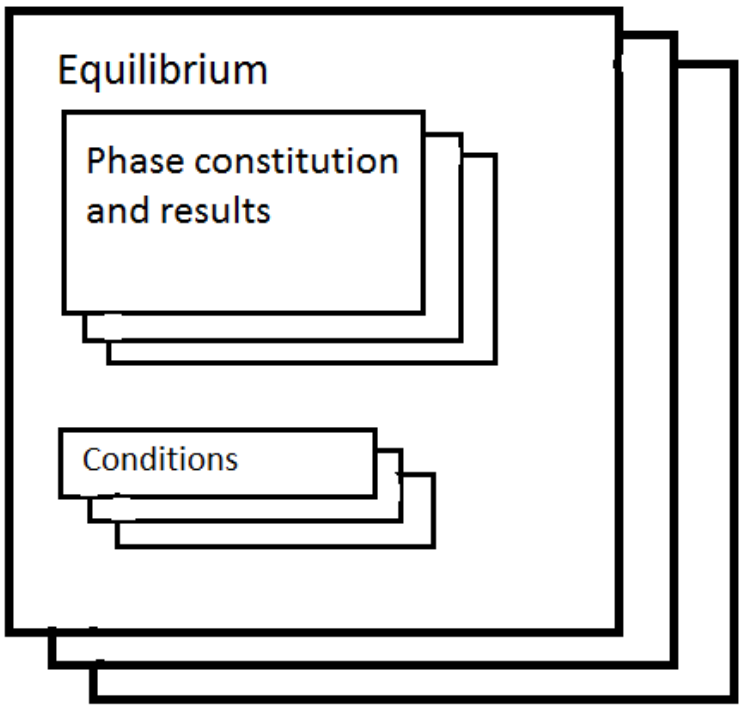


The amount and constitution of the phase varies with the external conditions like temperature and composition and are stored in the equilibrium record.

Parallel execution

Dynamic data



In addition to the dynamic phase data the current conditions are also stored in the equilibrium record. In simple cases there is just one equilibrium record but each is independent and several can be executed in parallel using OpenMP.

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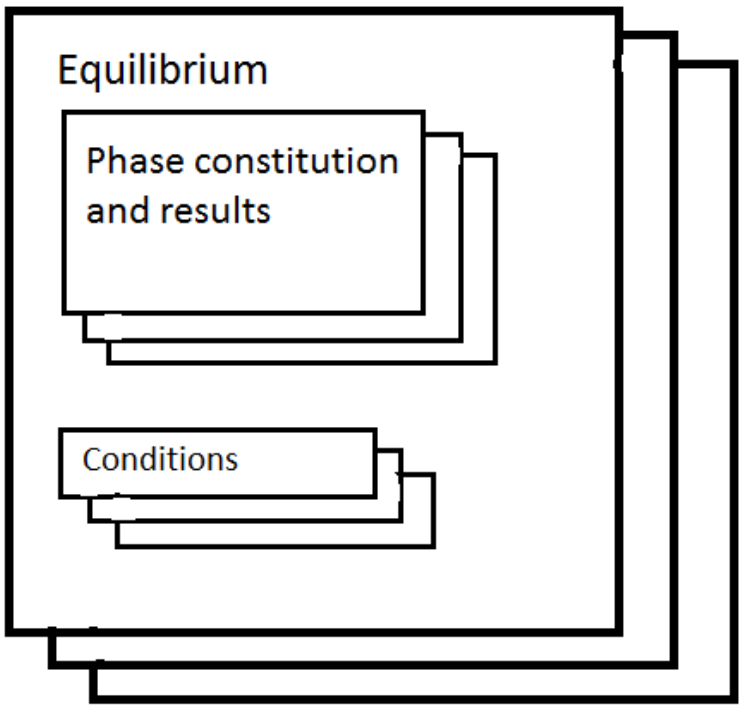
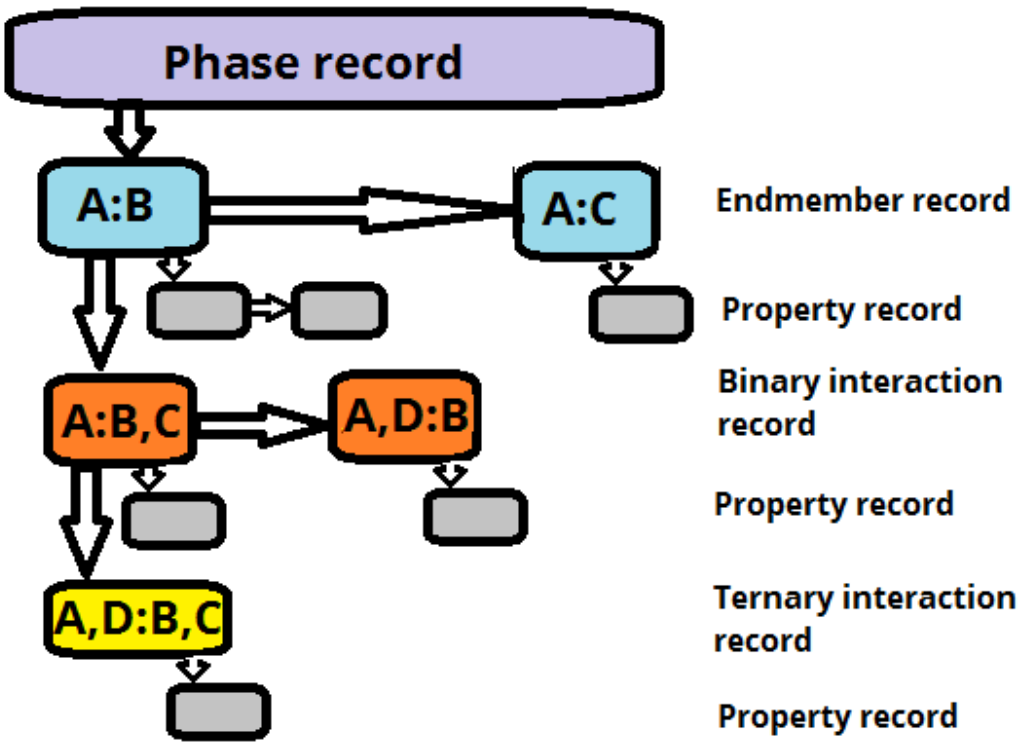


In addition to the dynamic phase data the current conditions are also stored in the equilibrium record. In simple cases there is just one equilibrium record but each is independent and several can be executed in parallel using OpenMP. This is useful for application software like assessment of model parameters using experimental and theoretical data and for phase field simulations when each gridpoint can have its own equilibrium record with a local set of conditions.

Separation of static and dynamic data

The Gibbs energy for a phase the with the model $(A,C)_a(B,D)_b$ may be:



This represent the equation

$$G = y_A y_B({}^\circ G_{A:B} + y_C(L_{A:B,C} + y_D L_{A,D:B,C}) + y_D L_{A,D:B}) + y_A y_C \, {}^\circ G_{A:C}$$

The model parameters are in the static data area and the constituent fractions, y_i and the results, G are in the dynamic data structure.

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- Command line user interface.
- A module for assessment of model parameters using experimental and theoretical data.

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- Command line user interface.
- A module for assessment of model parameters using experimental and theoretical data.
- Application software interface for using OC together with kinetic and other data.

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^{φ} and the total energy for the system is:

$$G(T, P, N_i) = \sum_{\varphi} \aleph^{\varphi} G_M^{\varphi}(T, P, y_i)$$

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The minimization procedure in OC is based on a proposal by Hillert in 1981 and its implementation in OC was published last year.
To ensure we find the global equilibrium there is an initial, optional, grid minimizer to calculate start values.

Application software interface, OCASI

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- A number of applications programs are provided with the source code.

Example 1 of use of OCASI, simulating uphill diffusion

At Ruhr University in Bochum, Germany, the ICAMS group has implemented OC in their free software for phase field simulations, Open Phase. As a test they have simulated the classical Darken experiment for "uphill diffusion" of carbon in two iron bars with almost the same carbon content but different Si and Mn content.

mass%	C	Si	Mn	Fe
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Si and Mn has opposite effects on the carbon activity, it is increased by Si and decreased by Mn.

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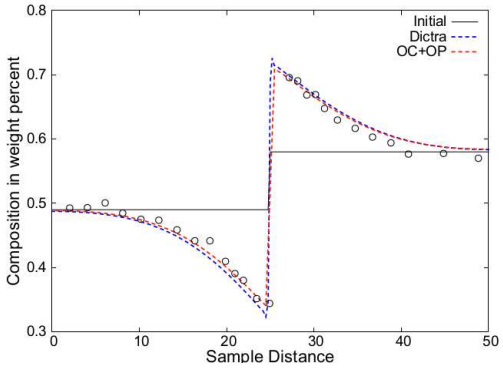

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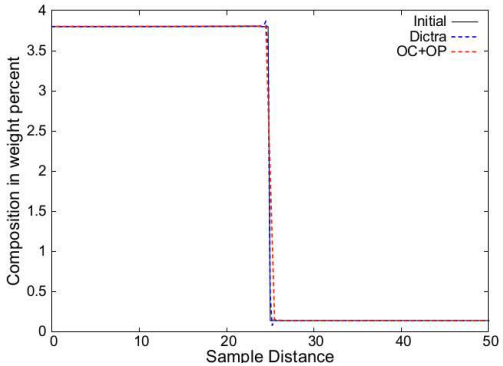

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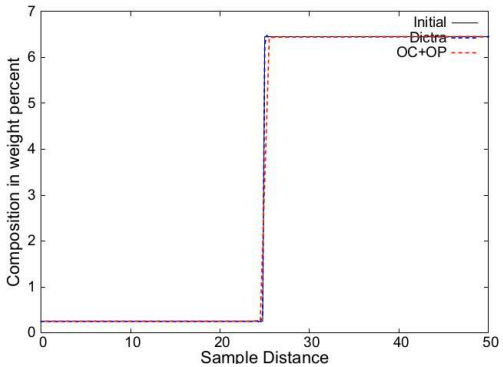

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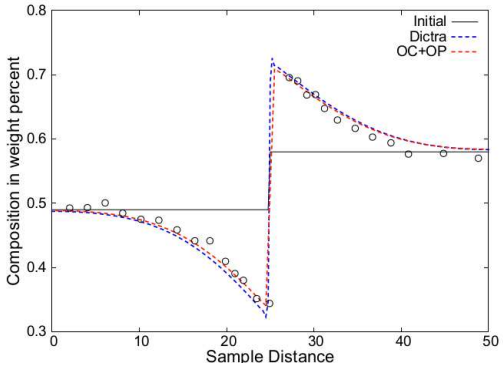

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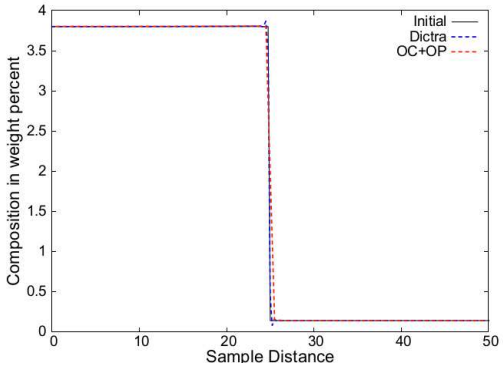

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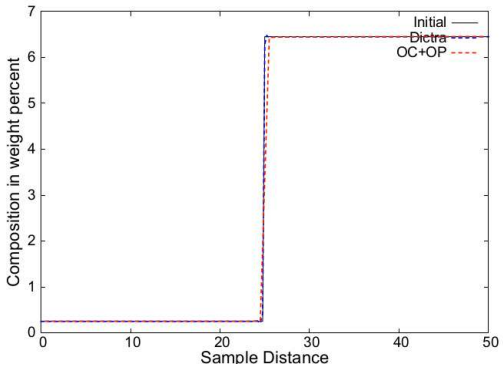

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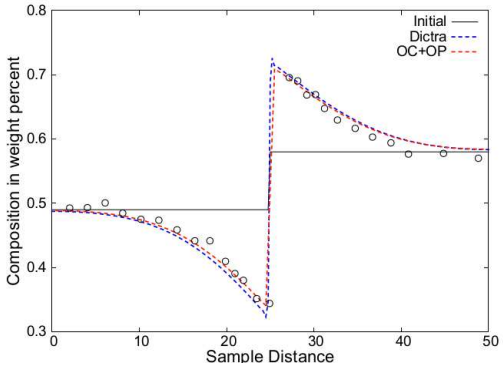

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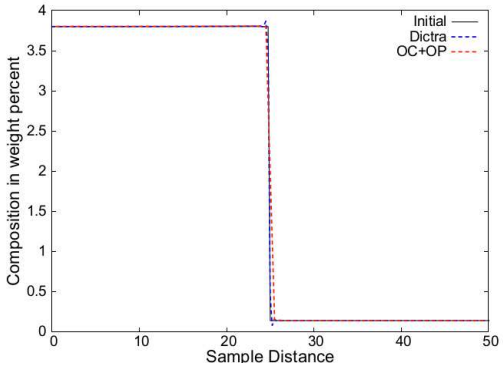

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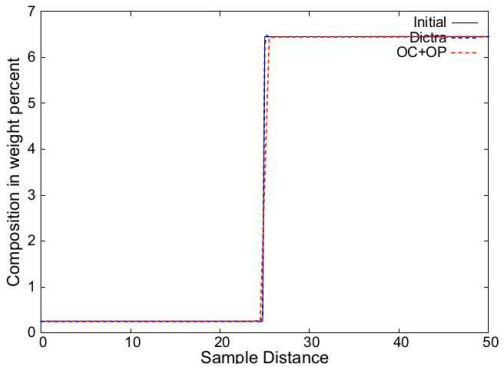

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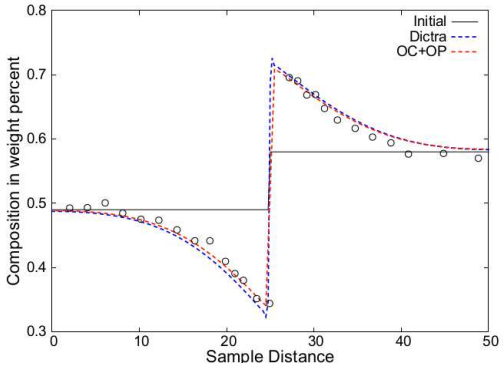

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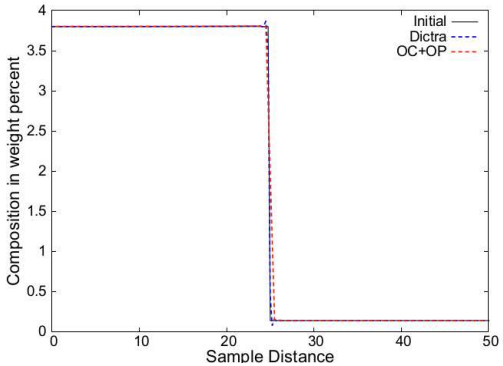

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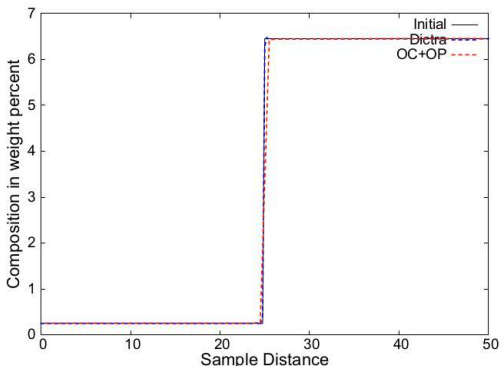

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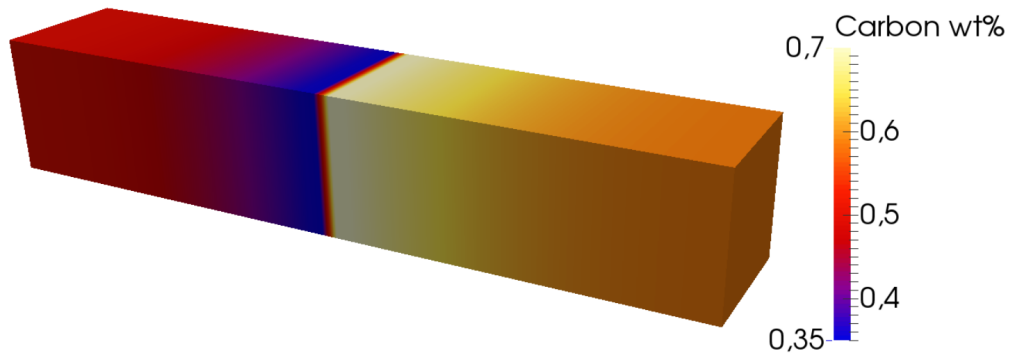
This is the simulated volume, the color show the C concentration.



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For 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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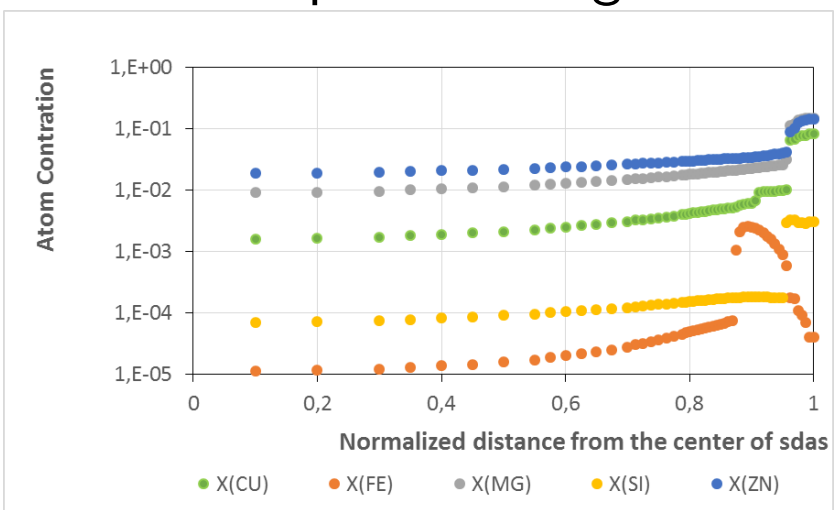

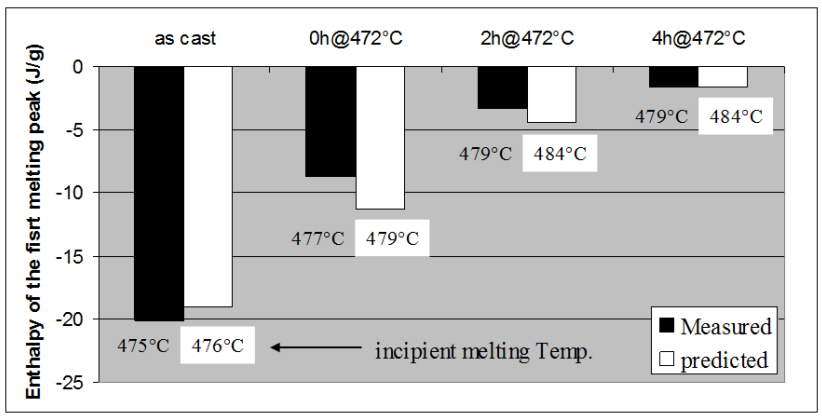

The left hand figure show the concentration profiles across a dendrite after solidification, the right the heat evolved during homogenization.

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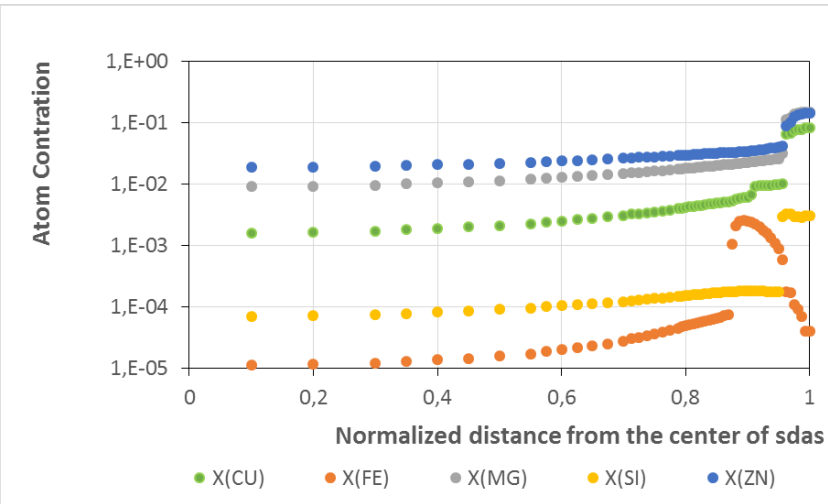

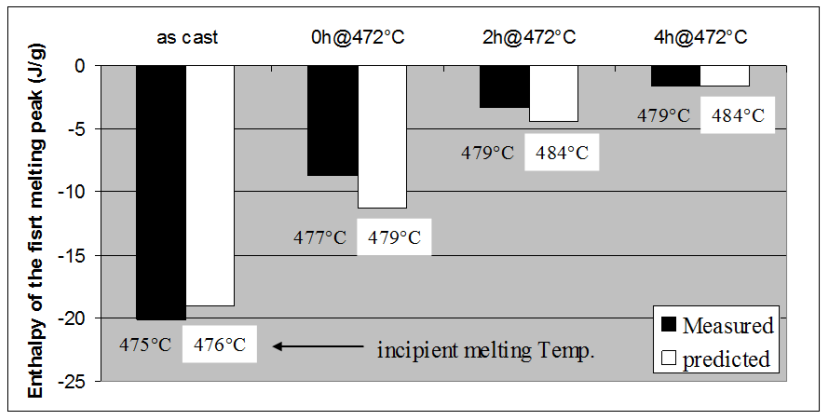

After implementing OCASI the same simulation took 3.5 hours using 12 CPUs in parallel, a gain of time with a factor of 24.

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As far as I know OC is the only thermodynamic software which can offer equilibrium calculations in parallel using the OpenMP library as a standard feature.

OCASI library, how to use?

An application program must first initialize the data structures before calling any routine in OCASI.

call tqini(n,ceq)

where n provides some dimensioning and ceq is a pointer initialized to point to an equilibrium data structure. This must be passed to all other routines. With another subroutine call one can create additional such pointers each representing a equilibrium with an independent set of conditions.

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The second step is to read the thermodynamic data from a database
call tqrpfil(database,nel,elnames,ceq)
just passing the database name, the number and names of the elements to select and the equilibrium record pointer. The database information is stored in the static data structure.

Phases and phase tuples

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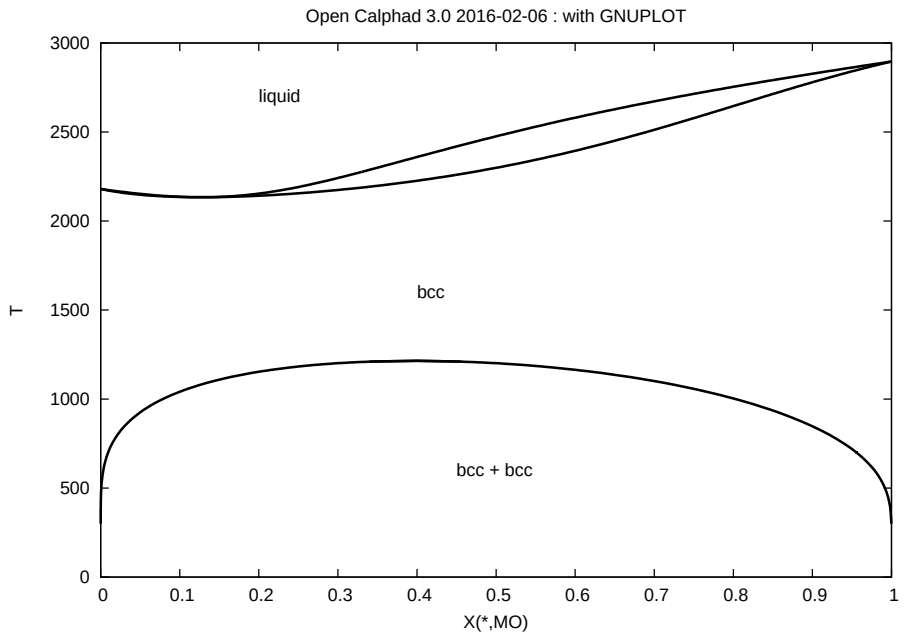

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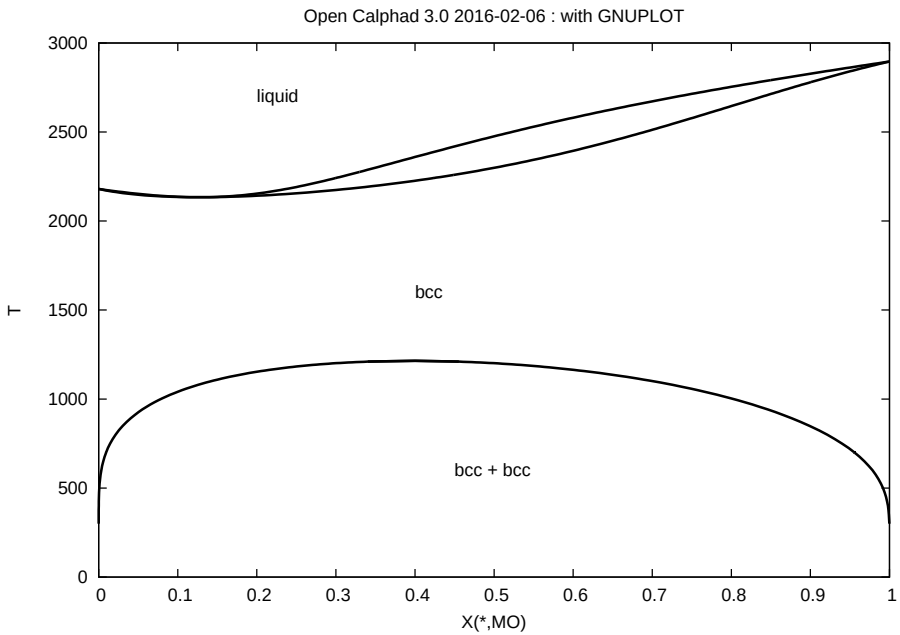

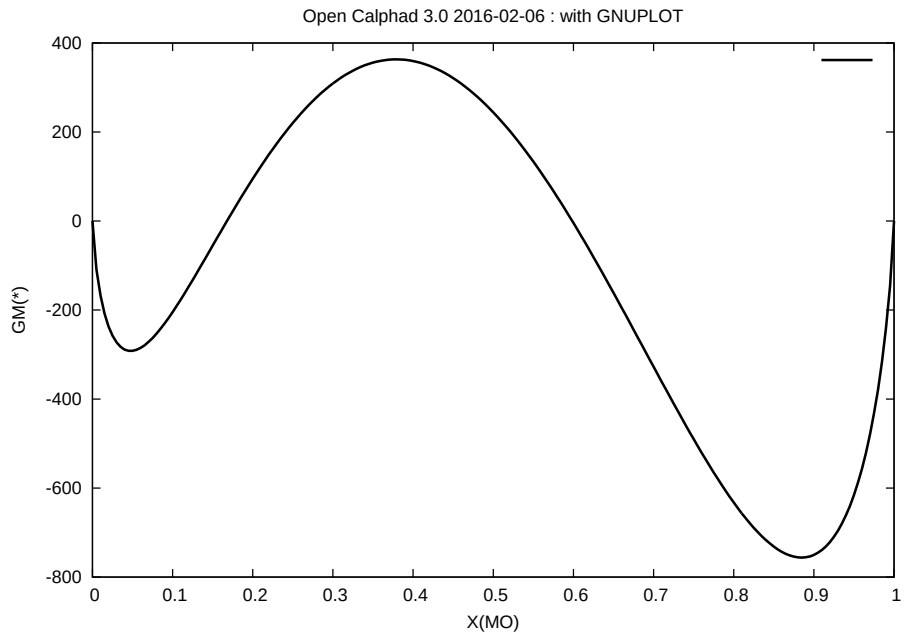

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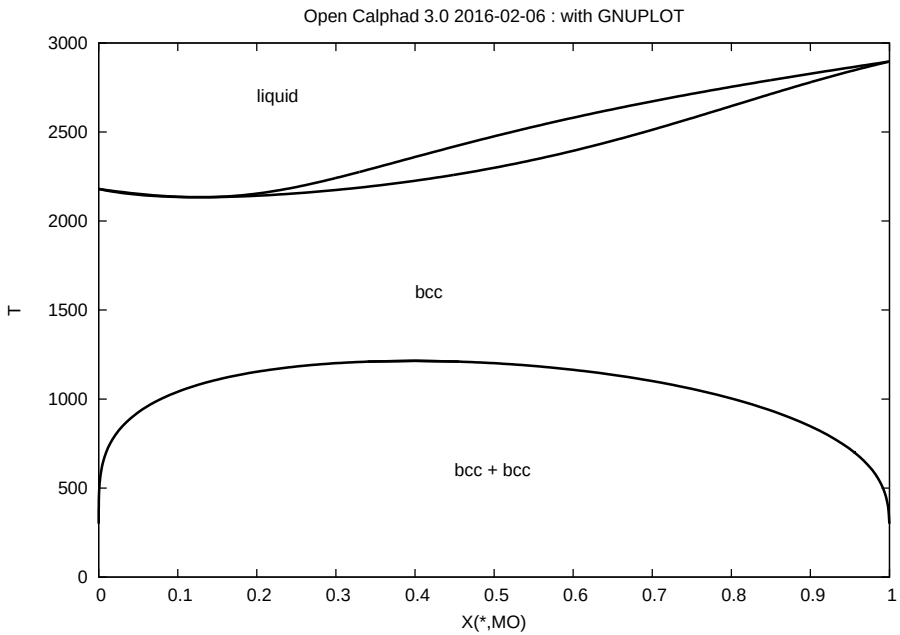

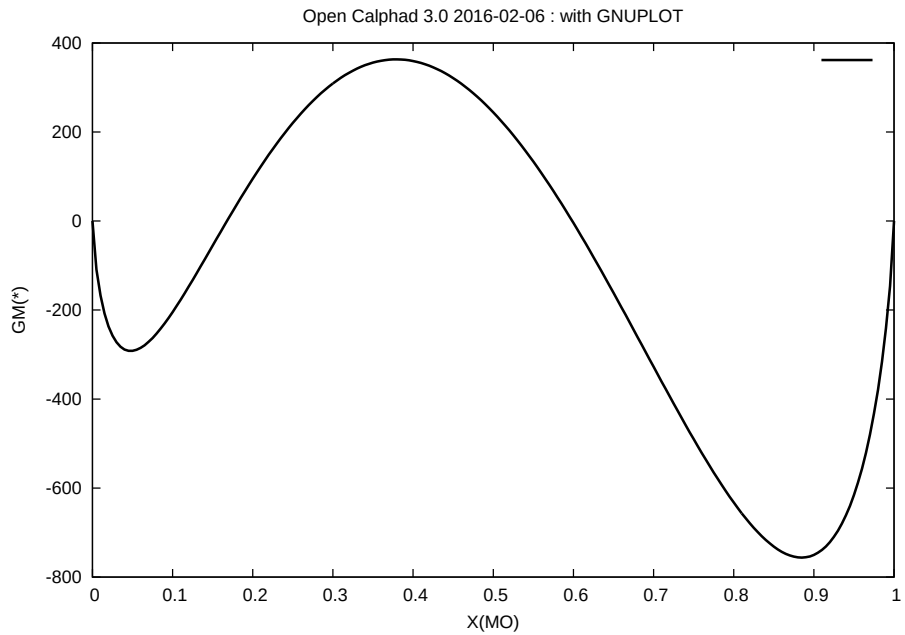

The right hand figure shows the Gibbs energy curve for bcc at 900 K with a convex part. As this is unstable the phase separates in two phases with the same structure but with different compositions. In OCASI these are treated as phase tuples with two indices, one for the phase, the other for the composition set.

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Each phase tuple has a complete set of dynamic data in the equilibrium record but all phase tuples for the same phase has the same thermodynamic description, the static memory does not change.

OCASI library, state variable symbols

State variables are important as they are used to set conditions and extract results. All state variables are identified by their symbols and most state variables have their "normal" symbols like T, P, V, N and X.

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These are just a few of the available state variables in OC.

OCASI library, setting conditions

To set a condition this subroutine is used.
call tqsetc(stv,n1,n2,value,cnum,ceq)
stv is a text with the state variable symbol like T or X or MU.
n1 and n2 are zero if not needed (like for T) but can be used for phase or component indices. Value is the value the state variable should have.
cnum is returned as an index of the condition.

Examples:
call tqsetc('T ', 0, 0, 1000, cnum, ceq)
call tqsetc('X ', 1, 0, 0.1, cnum, ceq)

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OCASI library, calculating equilibrium

In order to calculate the equilibrium the degrees of freedoms must be zero, i.e. the number of conditions must be equal to the number of components plus 2. The equilibrium is calculated with this call:
call tqce(target, n1, n2, value, ceq)

The **target** is an optional state variable name (with indices n1 and n2) and **value** is the desired value of this.
If you specify a target you should have one degree of freedom in the system and the software will try to adjust the system to reach the target value. This feature is mainly interesting when simulating a chemical process.

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If no target is specified a normal equilibrium calculation is made. There is an option to calculate the equilibrium with or without the grid minimizer.

OCASI library, extracting information

After a successful calculation you can extract values of all kinds of state variables with

call tqgetv(stv, n1, n2, n3, values, ceq)

stv, n1 and n2 has the same meaning as when setting conditions. It is possible to use -1 to indicate that you want all values of a state variable, for example all mole fractions.

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The amount of all phases:
call tqgetv('NP ', -1, 0, n3, values, ceq)
All mole fractions of phase with index 1:
call tqgetv('X ', 1, -1, n3, values, ceq)
Other modeled properties like the mobility of Fe in the BCC phase can be retrieved by the same subroutine:
call tqgetv('MQ&FE(BCC) ', 0, 0, n3, values, ceq)

Dynamic data: a phase data record in ceq

```
  TYPE gtp_phase_varres
! Data here are for a composition set of a phase in an equilibrium record, ceq
! phlink: is index of phase record (static data) for this phase_varres record
! phstate: indicate state: fix/stable/entered/unknown/dormant/suspended
! phtupx: phase tuple index
     integer phlink,phstate,phtupx
....
! yfr: the constituent fraction array
     double precision, dimension(:), allocatable :: yfr
...
! prefix and suffix are added to the name for composition sets 2 and higher
     character*4 prefix,suffix
...
! arrays for storing calculated results for each phase (composition set)
! amfu: is amount formula units of the composition set (calculated result)
! netcharge: is net charge of phase (must be zero for stable phases)
! dgm: driving force
     double precision amfu,netcharge,dgm
!   last index 1=G, 2=TC, 3=BMAG. Properties defined in the gtp_propid record
! gval(*,1): is G, G.T, G.P, G.T.T, G.T.P and G.P.P
! dgval(1,j,1): is first derivatives of G wrt fractions j
! dgval(2,j,1): is second derivatives of G wrt fractions j and T
! dgval(3,j,1): is second derivatives of G wrt fractions j and P
! d2gval(ixsym(i,j),1): is second derivatives of G wrt fractions i and j
     double precision, dimension(:,:), allocatable :: gval
     double precision, dimension(:,:,:), allocatable :: dgval
     double precision, dimension(:,:), allocatable :: d2gval
  END TYPE gtp_phase_varres
! an array of these records is allocated inside each equilibrium record, ceq
```

Dynamic data: iso-C binding and ceq

The fortran TYPE record can be summarized for C++ software by the ISO C interface as:

```
typedef struct {
int phlink, phstate, phtupx;
        ...
char prefix[4], suffix[4];
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double *yfr;
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The first and second derivatives of the Gibbs energy are calculated analytically by the model package and used in the minimization algorithm to handle conditions of different types, improve speed of convergence and stability.

OCASI library, using the Fortran data structure

Via the "ceq" pointer to the equilibrium record it is possible to access data directly inside the OC equilibrium record, without the use of subroutines and state variables.
For example Gibbs energy for a phase_varres record with index lokcs is
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Note that the partial Gibbs energy of a constituent is not the chemical potential. To obtain the chemical potentials from partials one must calculate an expression like this for a stable phase:

$$\mu_i = \left(\frac{\partial G}{\partial N_i}\right)_{T,P,N_7 j\neq i} = G_M + \left(\frac{\partial G_M}{\partial x_i}\right)_{T,P,x_{j\neq i}} - \sum_j x_j \left(\frac{\partial G_M}{\partial x_j}\right)_{T,P,x_{k\neq j}}$$

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The application software must never change a value inside the OC data structure. Setting conditions, constitutions etc. must always be made via calls as additional variables may need to be updated.

OCASI library, iso-C binding and ceq

Using OC for programs written in C++ is easy using the iso-C standard for transfer of data between C++ and Fortran. As the passing of arguments is different in C++ and Fortran one must have a separate set of routines, for example

- **c_tqini(n,c_ceq) bind(c, name=c_tqini)** to initiate OCASI
- **c_tqsetc(statvar, ... , c_ceq) ...** to set a condition
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Both the application examples shown were written in C++.
Based on Fortran and C++ compatibility, it is also possible to interface OCASI functionalities in the Java language thanks to the Java Native Interface. Or other popular software languages.
But Fortran is still a useful language for number crunching.

Heat capacity, the dot derivative

The heat capacity is not available as state variable and to obtain it OC has implemented the "dot derivative" feature developed by Bo Jansson in the Thermo-Calc software. The symbol "H.T" is

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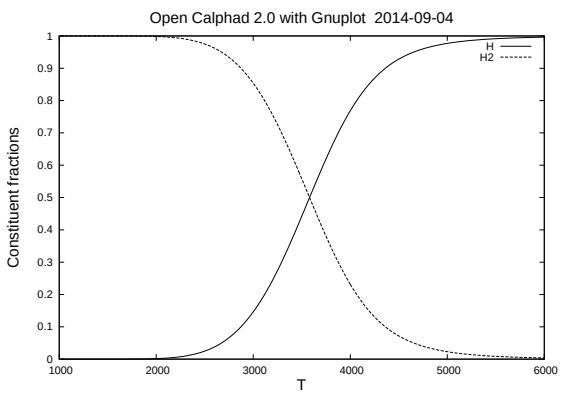
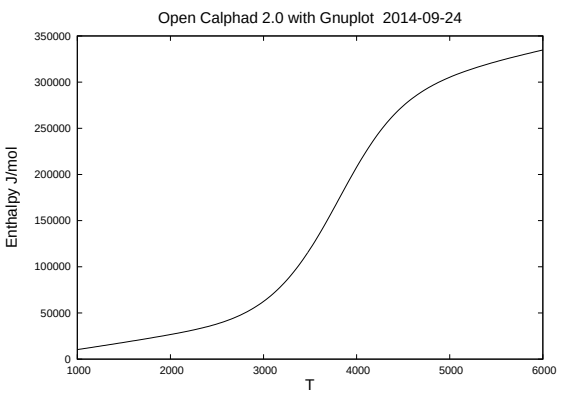
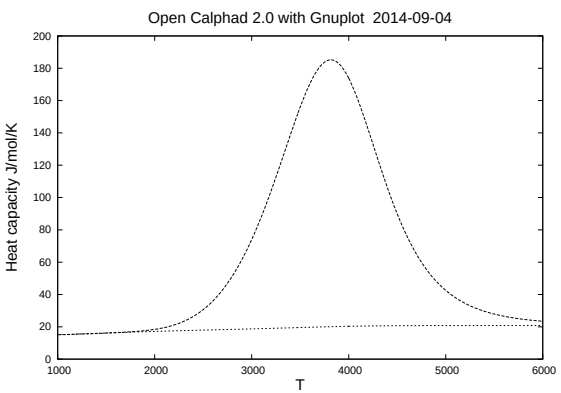
The heat capacity can be complicated to calculate when phases have internal degrees of freedoms as shown for a pure H gas with H_1 and H_2:







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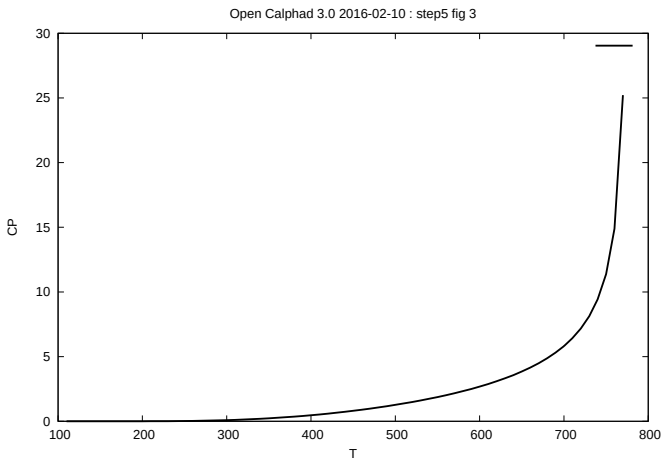
Order/disorder transitions and variable fractions of defects in solid phases have an influence on the heat capacity also. This is the heat capacity curve for the $L1_2$/A1 transition for $FeNI_3$



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The "dot derivative" in OC (and TC) is calculated using the second derivatives of G from the last equilibrium calculation, there is no need of any numerical derivation.
The second derivatives are also used to calculate the stability function and needed to transform mobility data to diffusion coefficients.

Other use of dot derivatives

Dot derivatives can also be interesting to calculate properties important for simulations like the slope of the liquidus surface

$$X(\mathrm{Liquid}, \mathrm{Cr}).T = \frac{\partial X_{\mathrm{Cr}}^{\mathrm{Liquid}}}{\partial T}$$

gives the change of the Cr content in the liquid with T (if there are also other phases stable).

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Without this facility one would have to calculate the slope by taking the difference between two equilibrium calculations with a small temperature difference.

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- The user interface is a command interface with macro facilities.
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But you can fix things yourself!

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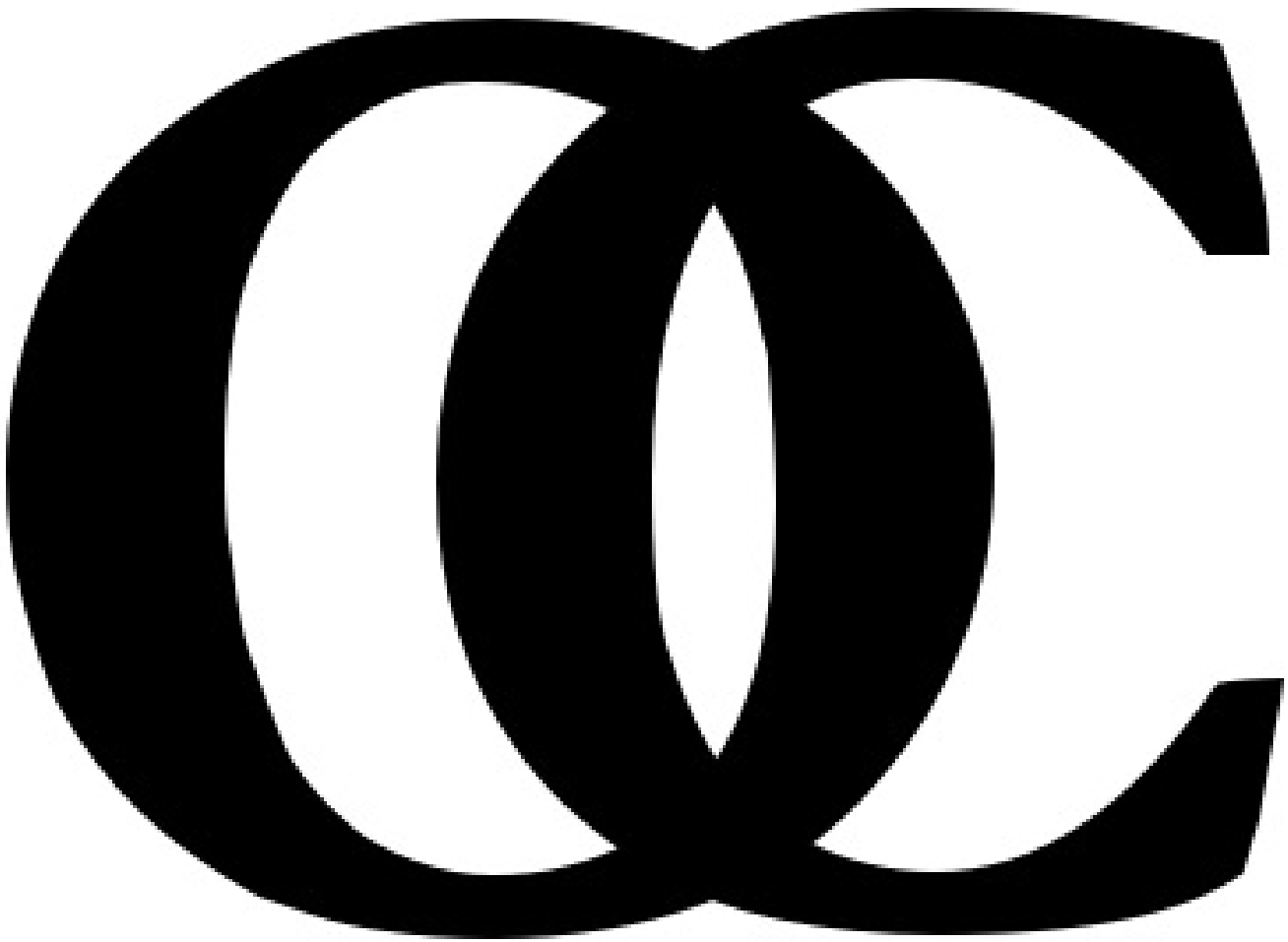

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Thanks for listening

Time left?

Algorithm for equilibrium calculation

maybe??