Getting started with OpenCalphad

Bo Sundman, August 4, 2018

Opencalphad (OC) is a free software with GNU GPL license. The last version is available at the following web site:
http://www.opencalphad.org or the

A development version is available at the opencalphad repository at::
http://www.github.com/sundmanbo/opencalphad

You can contact me at: bo.sundman@gmail.com

Please be aware that this software is under development. Your feedback about problems and errors is important to make it better. But if you have problems with the installation please contact a local expert.

OC cannot replace your favorite thermodynamic software today or tomorrow but the main advantage is that you have access to the source code and can (with some efforts) add or fix things yourself that you are missing in your favorite software.

There are several papers describing OC:

- **OpenCalphad - a free thermodynamic software**, Bo Sundman, Ursula R Kattner, Mauro Palumbo and Suzana G Fries (Open Access) Integrating Materials and Manufacturing Innovation (2015) **4:1** DOI 10.1186/s40192-014-0029-1
- **The implementation of an algorithm to calculate thermodynamic equilibria for multi-component systems with non-ideal phases in a free software**, Bo Sundman, Xiao-Gang Lu and Hiroshi Ohtani, Computational Materials Science, **101** (2015) 127-137.
- **The OpenCalphad thermodynamic software interface**, Bo Sundman, Ursula R Kattner, Christophe Sigli, Matthias Stratmann, Romain Le Tellier, Mauro Palumbo and Suzana G Fries, Comp Mat Sci, **125** (2016) 188-196

There is also an extensive documentation provided with the software:

- Getting started with OpenCalphad (this document).
- Install-OC, several different versions.
  - Install-OC-Windows-MinGW on Windows using MinGW.
  - Install-OC-Windows-Cygwin on Windows using Cygwin (in French).
  - Install-OC-Linux-or-macOS on Linux or macOS using GNU.

- news-OC5 about features and user interface.
- UG, User Guide and manual.
- OC-macros, examples how to use OC.
- GTP, General Thermodynamic Package describing the model package.
- HMS, Hillert's Minimizer describing the equilibrium calculations.
- SMP, StepMapPlot describing calculation and plotting of diagrams (draft).
- OCASI, OC Application Software Interface (draft).
- Assessments using OC (draft).

1 General information

There is no automatic installation routine for OC, you must download and compile the software yourself. You may also have to install Fortran compilers and the GNUPLOT software if you do not already have them. The OC development team cannot offer you any help for that, please ask some local experts if you need help.

- The code is written in the new Fortran standard and requires a compiler like GNU Fortran 4.8 or similar.
- The last release of the source code can be found as a zip file on http:://www.opencalphad.org.

  The last development version can be obtained as a zip file at the opencalphad repository on the http://www.github.com. On that site there is also a wiki for information, discussion and questions.
- See the special installation guides for advice on the installation. If you have problems please contact a local expert. This is all free software and we are not experts on hardware.
- If you have access to several CPUs you can test OC with parallelization using Open MP.
- In the "macro" directory there are examples for a variety of calculations.
- The TQ4lib directory has examples for using the software interface for Fortran and C/C++.
- Contributions of new and improved source code are welcome. You can do this by cloning the github repository. Contact Bo Sundman if you want to know more.

2 Some short hints to the user interface

See also news-OC and user guid (UG). The information in these (as well as this) files are not always up-to-date. You are welcome to inform me about errors and inconsistencies. If you do not like the current user interface you are welcome to develop your own.

2.1 Opening files with popup window

From version 5.018 I have added creating a popup window when opening a file (for a macro, a database or to save a calculation). In this window you can browse your directories to find the file. This has some consequencies for how to edit you macro files that you should be aware of.

You can turn off the open file popup window feature with the command *set advanced popup*. You can turn it on again with the same command.

- The directory where you start the session with OC is called the "working directory". On a linux system you can find this directory by typing "pwd" before starting OC (or if you type *@pwd* inside OC). On a Windows system you can see the working directory and its files if you type *@dir* inside OC.
- When the popup window is opened the directories and files matching the "filter" in the working directory are listed. The filter when open a macro file is "OCM" and when opening a database file it is "TDB" which means only files with these extensions are listed. You can change the directory in the popup window to select the file you want and you can read a file with another extension. OC will save internally the directory where you start the macro.
- Inside a macro file you normally read a TDB file and if you do not specify the name of the database on the same line as the command *read tdb* the popup window will open so you can specify the file in this window.
- But normally you know which database you want to use inside the macro and if you give the file name on the same line: *read tdb filename* the popup window will not open and OC will search for the specified database file starting from the "working directory". But if the database file is in the same directory as the macro file you MUST prefix "filename" with "./", i.e. *read tdb ./filename*. You may include directories in "filename", (including "../" to go to the directoty above). OC will replace the "./" by the directory where you started the macro or prefix "../" by this directory.
- In the macro file you can give the full path to the file to be opended but that is rather clumsy.

- When you open a file for write inside a macro, like output from a plot, you can also specify the file name in the command prefixed by "./" if you want to save the file on the same directory as the macro file. Otherwise it will be saved at the working directory.

- If you use the switch "/output=" or "/append=" after a command to redirect output from the command you can also use the popup window to specify the file name or use a filename with or without the prefix "./". The filter in this case is "DAT". (I forgot this in 5.018 so it will be available from 5.019 or later.)

You are welcome to provide feedback on this popup feature.

2.2 Entering and manipulating thermodynamic data

In this and the following sections you can find a brief and unstructured summary how to use OC and of the commands that may be useful.

- Thermodynamic data can be read from an unencrypted TDB file *read tdb "filename"* or entered interactively, see the *enter* commands. You can specify which elements you want from the TDB file but not select the phases. Phases you do not want you can suspend from the calculations with the command *set status phase ... = suspend*.

  If you already have data in the program and want to read new thermodynamic data from a file you must first remove the old data. You can remove all the thermodynamic data in the program by the command *new YES*.

- There are some exception from how data are entered into OC compared to Thermo-Calc, most important perhaps the "partitioning" of a phase into an ordered and disordered part. OC has implemented this in a different way and it is sometimes necessary to edit the TDB file before reading such partitioned data from a TDB file.

- You can save the thermodynamic data and results from a calculation (but not STEP and MAP results) on an unformatted file *save UNFORM "filename"* and read it back into the program with *read UNFORM "filename"*. But beware the format may change with a future release! The unformatted files may not be compatible with a computer with another operating system.

- You can save the thermodynamic data using the TDB format by a command *list data TDB filename*. The TDB format used by OC can, with some exceptions, be read also by other thermodynamic software which accepts TDB format.

- You can list the thermodynamic data on the screen with the *list data* command. You can list on a file by using the switch *list /output=filename ....* If you want to write a TDB file use the command *list data TDB*.

- You can enter thermodynamic data from a macro file as well as commands for calculations. In order to document errors or problems please send a complete macro file with data and commands reproducing the error to Bo.Sundman@gmail.com

  You can generate a macro file interactively by setting a log file *set log "filename"* and then (after some editing) use the log file as a macro with the extension OCM. The log file has the extension LOG.

2.3 Setting conditions

- To calculate you must set conditions on the external variables like temperature, T, pressure, P etc. The number of conditions must be equal to the number of components plus 2 (Gibbs phase rule).

- Setting conditions is similar to the Thermo-Calc software. Each condition is set separately by the command is *set cond "state variable" = "value"*. The safest set of conditions for calculating an equilibrium, i.e. which has most chance to converge, is to set values on T, P and N(element), i.e. the total amount of each element. The table at the end gives a list of available state variable symbols and their meaning.

- It is also possible to set conditions on chemical potentials, activities, enthalpies, volumes and that a phase is stable (fix). See the macro file examples how this is done. Note that some commands are fragile and they may also change between releases of the OC software, depending on new ideas and suggestions by users.

- The intention is that you should be able to combine any set of conditions to calculate the equilibrium, i.e. you should be able to combine conditions on mole fractions, mass fractions, fix phases, chemical potentials, enthalpies etc. For conditions on mole fractions you can also enter expressions as conditions, for example to calculate the congruent melting of UO_2 you can set a condition x(liq,o)-x(c1_mo2,o)=0 (see macro map4.OCM).

- For users with FactSage background there is a command *set input_amount* which allows the user to set the overall composition by specifying the amount of moles of different species in the system. The software converts this to *conditions* on the amounts of the components.

- You can only use components to set conditions on the amounts, activities and chemical potential. By default the components are the same as the elements but with the command *amend components* you can specify any orthogonal set of species as components.

  Beware that with other components than the elements your mole fractions and amounts of phases may be negative or larger than unity.

2.4 Calculation

- The command *calculate equilibrium*, which can be abbreviated *c e*, tries to calculate the equilibrium. As the minimizer needs a guess of stable phases and their start constitution, the OC software tries first to invoke a global grid minimizer to find such a guess. The grid minimizer requires that the conditions are T, P and overall composition (N, B, x or w).

- If you want to provide yourself a guess of the set of stable phases and constitutions you can use the *amend const phase "name" "amount" "constitution"* $\cdots$ followed by the command *calculate no_global*, abbreviated *c n*.

- The grid minimizer that calculates start points for the general minimizer is powerful but a bit primitive. If you have ideas how to improve it you are welcome to provide advice or code. There is a command to have a denser grid (about 10 times more grid points) using the command *set advanced dense*

- You should always check the results with you favorite thermodynamic software. Please give documented feedback on any differences.

- If the calculation does not converge directly try to use the command *"c n"* two or more times to continue to iterate from the set of phases you have. The *"c e"* command will run the grid minimizer and, therefore, will normally give the same result each time.

- You can also try to change the number of iterations and convergence criteria with the command *set num "max iterations" "convergce criteria"*. Default values of these are 500 and 10^{-6}.

- If everything fails try to simplify the conditions for a first calculation. The simplest are values of T, P and N(component). When that has converged change the conditions one by one to those you are interested in and for each change calculate without the grid minimizer, i.e. using *"c n"*. Calculations at temperatures and compositions where the system is single phase have a higher chance of success. The algorithm to change the set of stable phases is fragile and is still being fine-tuned.

- Phases with miscibility gaps can be a problem. The grid minimizer should detect such and automatically add new composition sets for phases that can be stable with two different compositions. Composition sets created automatically have the suffix AUTO.

- The user can also add composition sets manually with the command *amend phase "name" comp_set* . You can add a prefix and suffix (max 4 letters) to the phase name (for example the cubic carbide treated as a composition set to the FCC phase can have the prefix MC so the full name is MC_FCC.

  Composition sets have a number after the phase name preceded by the letter #, like LIQUID#2. The user can use both pre- and suffixes or use the composition set number to specify the composition set. A phase can have up to 9 composition sets.

- When entering a composition set manually you are asked for a min or max values of each constituent. After a calculation the software will try to match a calculated constitution of a phase which has several composition sets to the set with the closest default constitution.
- To set the default constitution of the first composition set use *set phase "name" default_constitution* $\cdots$.
- There are several options to calculate things:
  - *calculate all* calculates all equilibria set by the set range command. It is intended for equilibria with experiments and used in assessments but can be used to calculate a range of equilibria not suitable for the STEP command.
  - *calculate global_gridmin* will use the global gridminimizer and not the final iterative routine,
  - *calculate phase* to calculate properties for a specific phase. You must first specify the amount of the phase and if you want to use the current constitution. Then you can select
    - *only G* to get G and derivatives with respect to T.
    - *G and dGdy* to get G and also first derivatives w.r.t. constituents.
    - *all derivatives* to get G and all first and second derivatives w.r.t T, P and constituents.
    - *constitution adjustment* This will ask for a new composition (default is the current or the one specified) and miminize the Gibbs energy of the specified phase to have the equilibrium constitution (for example adjust the fraction of gas constituents or sublattice fractions). It will return the value of G and all chemical potentials (divided by RT).
    - *diffusion coeff* This will also ask for a new composition and return the values of the Darken stability matrix calculated as $\frac{\partial G_{\mathrm{A}}}{\partial N_{\mathrm{B}}}$ and if the phase has any mobility data also their values.
  - *calculate symbol* will calculate the value of one or more symbols.
  - *calculate tp_funs* will calculate the value and the first and second derivatives with respect to T and P for all tp functions (used for the model parameters).
  - *calculate transition "phase" "condition"* calculates the value of the "condition" when the phase is just stable, for example the melting T if the "phase" is LIQUID.

2.5 Setting the status of phases: entered, fixed, dormant, suspended

To set the status of a phase to be fixed is treated as a condition.

- By default all phases have the status ENTERED. You can suspend phases you do not want by *set status phase "name" ··· = "suspend"*.

  If the phase should be stable you will calculate a metastable equilibrium.

- To specify that a phase must be stable you can set its status to fix, the command is

  set status phase "name" = "fix" "amount".

  If the amount is set to zero OC will calculate a point on the solubility line of the phase. Note it may fail because there is no such point due to the other conditions.

- The dormant status means the phase cannot be stable but its driving force is calculated. If this is positive the phase wants to be stable and the calculated equilibrium is metastable.

2.6 Listing many things

Most listing are written on the screen but when output obviously should be written on a file the program will ask for a file name. If you want the output from other listings to be written on a file you can use the switch */output=filename* or */append=filename* directly after the first command. For example *list /out=result r,,,*. The extension of the output file will be DAT. The output file will be reset to the screen after each command.

There is also a SAVE command mainly intended for saving on a file. For example *save tdb filename* will write all the thermodynamic data in the OC TDB format on the file with the extension TDB. This can be read back later as a TDB file.

- Listing results after a calculation is done by *list result "option"*. This is the default list and can be abbreviated *l,,*. This list will always include the current conditions and some global results and one line for each component. The options are at present:
  - 1 list of stable phases with amount and composition in mole fractions in value order.
  - 2 list of stable phases with amount, composition and constitution in mole fractions in value order.
  - 3 list of stable phases with amount and composition in mole fractions in alphabetical order.
  - 4 list of stable phases with amount and composition in mass fractions in value order.
  - 5 list of stable phases with amount and composition in mass fractions in alphabetical order.
  - 6 list of stable phases with amount and composition in mass fractions and the constitution in value order.

  - 7 list of all phases with amount and composition in mass fractions in value order.
  - 8 list of all phases with amount and composition in mole fractions and constitution in alphabetical order.
  - 9 list of all phases with amount and composition in mole fractions and constitution in value order.

- The *list short A* gives one line for each component, species and phase. In this list you may note the use of the "phase tuple" to indicate composition sets. A phase tuple has two values, one is the phase number, the other the composition set number. The first composition set of a phase has the same tuple number as the phase number. As composition sets can be added and deleted the tuple number of a higher composition set may change.

- The *list short P* gives one line for each phase, separated in stable, entered and dormant, listed in order of increasing instability (driving force).

- The *list bibliography* list all or a single bibliographic reference. Bibliographic references are entered when entering parameters. The *amend biblio* allows interacting amending of the bibliographic item.

- The *list data screen* lists all thermodynamic data with bibliographic references. Note this output is not the TDB format.

- The *list equilibria* list all entered equilibria (not any results). By default there is only one equilibrium but during step and map each node point is entered as an equilibria. The user can also enter equilibria manually.

- The *list model_param_id* list all symbols for which one can enter parameters. By default the G is Gibbs energy, TC the combined Curie and Neel temperature etc.

- The *list phase* has several options to list various data for a phase.

- The *list state_variables* lists individual values of state variables. The wildcard character "*" can be used for "all". Terminate with an empty line.

- The *list symbols* list the symbols and their expressions. There two predefined symbols, R and RT. The user can enter any number of additional symbols as functions of state variables or other symbols. To calculate (and list) the value of a symbol use *c sym*.

- The *list tp_symb* lists the functions entered for the model parameters. To calculate their current values use *c tp*.

2.7 Calculating and plotting diagrams

This part is unfinished and very rudimentary.

- You can calculate property diagram (one independent axis variable) or phase diagrams (two or more independent axis variables). The command to set an independent axis is

  set axis 1 "state variable" "min value" "max value" "increment". The state variable used must be a condition. Axis 1 and 2 are implemented.

- With one axis the *step* command will step from the current equilibrium to the max and min axis values.

- With two axis the command *map* will follow "zero phase fraction" (ZPF) lines within the limits of the axis by replacing one of the axis condition with a phase fix with zero amount. In this way phase diagrams for any number of components can be calculated. While following such a line other phases may become stable or disappear and this generates a node point where several lines meet.

- Plotting of diagrams relies on GNUPLOT, a free software you can install from the web. The command *plot* asks for two axis variables and generates pairs of values from the results calculated by step or map commands.

  There are several options to the plot command that are demonstrated by the macro files.

- Macro files are easily created by using a log file while running OC interactively. On the log file all input (as well as default values) are written. Then you can edit this and finish it with the *set interactive* command to give command back to the keyboard.

  When you report problems or errors always sent a macro file that reproduces the error. Please try to find the simplest case that contains the error.

3 GNUPLOT graphics

OC uses the free GNUPLOT software to plot on the screen and other devices. You must install GNUPLOT before you can obtain any figures.

You can find GNUPLOT at http://gnuplot.info/download.html

In OC you can list or enter a GNUPLOT terminal by the command:

—>*OC5:* **enter gnuplot_term**

```
GNUPLOT terminals are: 5
 1  SCREEN   > set terminal wxt size 900,600
 2  PS       > set terminal postscript color solid fontscale 0.8
```

```
 3  PDF      > set terminal pdf color solid size 6,4 enhanced fontscale 0.45
 4  GIF      > set terminal gif enhanced fontscale 0.7
 5  PNG      > set terminal png enhanced fontscale 0.7
Enter or change a GNUPLOT termial
Terminal id (8 chars):
```

The terminals listed above are the default on Windows. On a Linux system they may be different. Before changing anything you should first start GNUPLOT and use the command **"set term"** to list the available terminals on your installation of GNUPLOT.

In OC after giving a PLOT command and specified your axis you can select to plot on any of the the terminal devices listed above (or which you defined yourself) by:

Options? /RENDER/: **graphics_format n**
where the number "n" is the gnuplot terminal you wish to use. If you wish to plot on SCREEN you do not need to give this command.

4 A summary of state variables.

The state variables are very important for setting conditions and listings. Those recognized by OC are given in table 1.

The state variables in the user interface have their common symbols, T for temperature, P for pressure, N for the total amount of moles, "N(element)" for the amount of moles of a component, "X(element)" for the mole fraction "MU(element)" for the chemical potential, "AC(element)" for the activity. The symbol B is used for the total mass (copied from the Thermo-Calc software), "B(element)" for the mass of an element and "W(element)" for the mass fraction. There are many more state variables like H, G etc, see the table, but not all of them can be used as conditions.

5 Phase status

You can specify that a phases should be stable by the command *set status phase* $\cdots$. For example to calculate the melting point of an alloy after specifying the composition and making a calculation at fixed T and P, you can give the commands *set cond T=none; set status liquid=fix 0; c n.* (The commands must be given on separate lines). You can also use the command *calculate transition* $\cdots$.

Table 1: A very preliminary table with the state variables and their internal representation. Some model parameter identifiers are also included. The suffix "z" in Sz etc is the optional normalizing letter M, W, V or F. The suffix S can also be used to indicate SER as reference state. The "phase" index for MU etc can be used to specify the reference state.

Symbol	Id	Index 1	Index 2	Normalizing suffix	Meaning
Intensive properties					
T	1	-	-	-	Temperature
P	2	-	-	-	Pressure
MU	3	component	-/phase	-	Chemical potential
AC	4	component	-/phase	-	Activity
LNAC	5	component	-/phase	-	LN(activity)=MU/RT
Extensive and normalized properties					
U	10	-/phase#set	-	-	Internal energy for system
UM	11	-/phase#set	-	M	Internal energy per mole
UW	12	-/phase#set	-	W	Internal energy per mass
UV	13	-/phase#set	-	V	Internal energy per m^3
UF	14	phase#set	-	F	Internal energy per formula unit
Sz	2z	-/phase#set	-	M/W/V/F	entropy
Vz	3z	-/phase#set	-	M/W/V/F	volume
Hz	4z	-/phase#set	-	M/W/V/F	enthalpy
Az	5z	-/phase#set	-	M/W/V/F	Helmholtz energy
Gz	6z	-/phase#set	-	M/W/V/F	Gibbs energy
NPz	7z	phase#set	-	M/W/V/F	Moles of phase
BPz	8z	phase#set	-	M/W/V/F	Mass of phase
Qz	9z	phase#set	-	M/W/V/F	Stability of phase
DGz	10z	phase#set	-	M/W/V/F	Driving force of phase
Nz	11z	comp/phase#set	-/comp	-	Moles of component
X	111	comp/phase#set	-/comp	0	Mole fraction
X%	111	comp/phase#set	-/comp	100	Mole per cent
Bz	12z	comp/phase#set	-/comp	-	Mass of component
W	122	comp/phase#set	-/comp	0	Mass fraction
W%	122	comp/phase#set	-/comp	100	Mass per cent
Y	130	phase#set	const#subl	-	Constituent fraction
Some model parameter identifiers					
TC	-	phase#set	-	-	Curie temperature
BMAG	-	phase#set	-	-	Aver. Bohr magneton number
MQ&X	-	phase#set	component X	-	Mobility of X
THET	-	phase#set	-	-	Debye temperature

6 Manipulating the source code

The OC software is provided with a GNU license which means that you have the source code and can use it and modify it as you wish as long as you do not try to make money of

it. If you want to include the OC software in a commercial program you must contact the copyright owners.

There is a fairly extensive documentation of the source code in the directory "documentation" and if you look at the code itself there are some comments there too. I have spent a lot of effort to make the data structures general and flexible to handle multicomponent and multiphase systems. But there was quite a lot of redundancy introduced during the development that eventually will be removed.

The set of subroutines is less structured and one problem has been that this code was my first attempt to use the new Fortran standard so there are probably many things that can be made simpler. You are welcome to point out where this can be done.

7 Application software library, OCASI, iso-C compatible

There is an OC Application Software Interface (OCASI) following the TQ standard to make it possible to use OC from application programs. The subroutines in this interface can be found in the directory "TQ4lib" together with a few test program. Read the separate readme files in these directories to compile and run these.

There is a Fortran version of the TQ library and also an iso-C version that can be called from C++/C routines. The isoC binding makes it possible to access data directly from the data structures defined inside the OC software. There are some test programs for this also.

Use only subroutines in the TQ library to access the OC software, do not call directly subroutines inside the OC code as they may not be available or have different functionality in a future release. If you miss some routines please sent a message or discuss this on the github wiki.

8 Parallelization

The code has been developed with parallelization in mind and I have now started to test this code and surprisingly it seems to work quite well. There is a macro parallel2.OCM showing a calculation of 400 different equilibria in a 6 component alloy. They need to be initialized which makes me a bit suspicious but testing changing some and calculate again seems to work. I have tested on a PC with 4 CPU and 8 threads and the clock time is about 3.5 times faster compared to calculate them sequentially.

Parallelization can be implemented in several levels in OC, for example the grid minimizer or even inverting the phase matrix, but the ability to calculate many separate equilibria in parallel is a key feature to implement full thermodynamic calculations for simulations of phase transformations using phase field and similar techniques.

Have fun and help make OC useful!