Installation of OpenCalphad on Linux

Bo Sundman, September 20, 2016

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 descrcipton below applies when installing OC on a "vanilla" Linux system, the guides available are:

- Install-OC-Windows-MinGW
- Installation de OC sous Windows avec Cygwin (in French)
- Install-OC-Linux

Step by step installation:

- The code is written in the new Fortran standard and requires a compiler like GNU Fortran 4.8 or similar.
- If you have not already installed a Fortran compiler you can get the GNU Fortran suite free from https://SourgeForge.net or some similar site. If you have Intel or another Fortran compiler you must be sure it is compatible with GNU Fortran 4.8 or later.
- Rename the file "Makefile-sequential" to Makefile
- If you have access to several CPUs you can test OC with parallelization using Open MP. In that case you should rename "Makefile-parallel" to Makefile
- Run the make command in a terminal window.**If you have errors running the make command files please contact a local expert.**
- For the graphics you must download and install the free GNUPLOT software, for example from SoureForge.

  Make sure your PATH includes the directory with the GNUPLOT program. If you do not know how to set your PATH ask a local expert.
- There is a documentation directory with several PDF files. Read the "Getting_started" documentation to understand how to operate the program. Also look at the "OC-macro" documentation which describes several macro files which you have on a directory "macro". These are useful to test the software and gives some ideas how to use it. There is also a news-OC4 for a summary of the features of OC.

- There is also a preliminary user guide "ochelp4" in the manual directory. The user guide is also available in the file "ochelp.hlp" in LaTeX format because it is used for the on line help. The user guide is still very primitive as many commands are changing or not yet implemented.
- The source code is in the directories "minimizer, models, numlib, stepmapplot, userif" and "utilities".
- The documentation of the source code is in the directory "documentation" in several PDF files: "gtp3" for the model package and "hms2" for the minimizer. The other software documentation, "smp2" for the step/map/plot routines, "assess" for the assessment module and "ocasi" for the application software interface are very preliminary.
- The TQ4lib directory has a few examples for using the software interface for Fortran and C/C++. An attempt to implement isoC binding to C++ has been made. Consult the "readme" files on the different directories how to install them.
- Contributions of new and improved source code are welcome. You can do this using the github repository. Contact Bo Sundman if you want to know more.
- The OC command line interface has a "VAX/VMS" flavor which reflects the age of the developer. It means the commands are "verbs" like *set, list, calculate, enter* etc. After the verb several objects are usually possible like *Set condition/status* etc. There is some redundancy so the same effect can sometimes be achieved by different combinations of verbs and objects.

  Each command and subcommand can be abbreviated, usually 3 characters are sufficient.

  If you want a graphical user interface you are welcome to develop it.

You are welcome to provide a better installation guide also!

Have fun and help make OC useful!