First install of OpenCALPHAD (=OC) under MS-WINDOWS

P Zeller - 21 septembre 2016

Context : OpenCALPHAD is an "open source" software written in fortran. It is up to the user to build an executable by compiling the source.
OpenCALPHAD also needs GNUPLOT.
This document describes one way to install the code in order to use it through the Windows command shell "cmd". It is suitable for a new user who has no experience in code compilation under Windows.

Warning *: This document IS NOT an "installation manual", but an ACCOUNT of my own experience. I do not guarantee that the reader will be able to reproduce the result. In particular he will most probably have to change downloaded filenames, either because his or her initial configuration is not similar to mine, or because filenames include a release number.*

1 Before starting to install

1.1 Initial configuration of the PC

NB : this is not really a choice : what follows is the configuration of my PC. The reader may have to adjust the rest of the document depending on his own configuration.

OS	Windows 7 Enterprise Service Pack 1, Système d'exploitation 64 bits.
GNUPLOT	If it is not already installed, start with "installing GNUPLOT" and then come back here (by pressing "Alt-left"... if MS-WORD is properly configured).

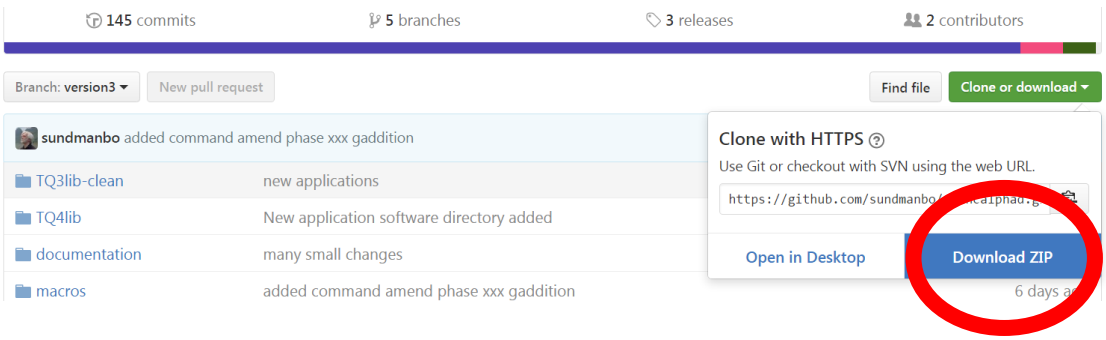
This procedure requires a knowledge of the Windows command shell "cmd"

This procedure requires a knowledge of how to "modify environment variables" in Windows.

1.2 Downloading OpenCALPHAD

Option	**Preference order**	
github (`https://github.com/sundmanbo/opencalphad`)	1	frequently updated
opencalphad.com	2	last stable version

Download the zip archive :



Extract in a folder like "C:\OPENCALPHAD" or any other folder whose name does not include any blank space character.

1.3 Choice between sequential or parallel code

Planned use	**Option to choose**
Command line calculations	***sequential*** or ***parallel***
Interfacing with another code (phase field, diffusion, thermomechanics, ...)	***parallel***
	OCASI install (= OC Application Software Interface)

NB :

- *For a new OpenCALPHAD user the sequential version offers no advantage compared to the parallel version. It is neither easier nor quicker to install.*
- *The sequential version may only be useful for an experienced user who only wants to **update** (and of course already has an operational compiling environment).*
- *This document gives no indication for installation of OCASI.*

1.4 Choice of the compilaation and execution environment

Option	**Advantages**	**Drawbacks**
MinGW version "0.6.2-beta-20131004-1"	Uses a Windows command shell (= no need to learn Linux shell language)	1. Reserved to "opencalphad sequential" because **buggy** environment. 2. May require editing OC *.F90 source files for compilation to succeed. 3. Impossible de compile the parallel version.
cygwin ou **cygwin/X**	1. Very **robust** tool: no problem either for installation or at runtime. 2. The graphical terminal (xterm) is much more powerful and user-friendly than the Windows command shell 3. The OC executable can be used both in a cygwin or a Windows terminal.	Requires learning the basic commands of the Unix/Linux shell language : cd, ls, cp, mv, rm, ...
MSYS2 version "msys2-x86_64-20160921"	1. Very recent gcc version (6.2.0). 2. The OC executable can be used both in a cygwin or a Windows terminal.	1. Requires learning the basic commands of the Unix/Linux shell language : cd, ls, cp, mv, rm, ... 2. Installing MSYS2 is a bit difficult due to a number of "**traps**" (not to call them bugs!)

NB :

1. *Whatever option is chosen the compiler will always be some flavour of "mingw", i.e. the gcc family (=GNU Compiler Collection https://gcc.gnu.org/) configured to produce binary executables natively running under Windows. For parallel libraries it uses DLL from Microsoft.*
2. *Bugs mentioned in this section may disappear in future releases of MinGW et MSYS2. New bugs may also appear. It may be that the users community for MinGW and MSYS is not as large as that of cygwin, so that cygwin ends up being much more robust ?*
3. *I also tried another option: compiling with native gcc in cygwin (gcc-core package, as opposed to mingw64-i686-gcc-core). This produces a parallel executable that performs very badly in terms of parallelism and is not even as fast as the sequential binary.*

4. *There may be other versions of MinGW and/or MSYS I'm unaware of ?*

My preference clearly goes to option #2 = "cygwin/X".

Continue by clicking on one of the following links :
Installing parallel OC under Cygwin/X
Install de parallel OC under MSYS2
Install sequential OC under MinGW

2 Installing parallel OC under Cygwin

To check whether cygwin is installed : Start Menu / enter "cygwin" in the search box.

If cygwin is installed : go to update
If cygwin is absent : go to install

2.1 If cygwin is already installed : update

Just check that all necessary packages are present, and install if not.
NB :

- to check for package presence when part of the name is known (e.g. *gcc*) :

```
cygcheck -c -d | grep gcc
```

As for compilers, in order to check whether viable alternative packages such as mingw64-**i686** instead of mingw64-**x86_64** are installed :

```
cygcheck -c -d | grep mingw64-i686-gcc-core
```

If they are, no need to add or replace as they are completely suitable (and produce exactly the same OC executables).

- Then to see the content of a package (list of included commands), e.g. :

```
cygcheck -l mingw64-i686-gcc-fortran
```

- Finally, to check both presence and version (e.g. for gcc or gnuplot), enter

```
gnuplot --version
```

or

```
x86_64-w64-mingw32-gfortran --version
```

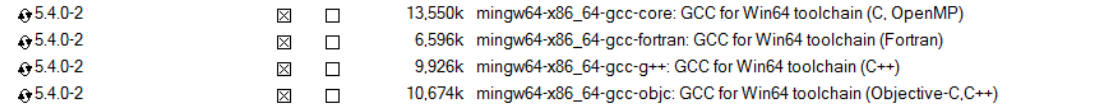
List of necessary packages : see here.

2.2 If cygwin is not present : install

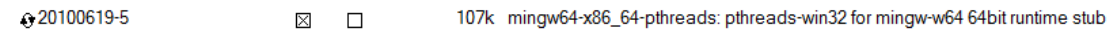
From site http://cygwin.com download **setup64.exe**, i.e. the 64-bit version, and save in C:\CYGWIN_annex.
Make a shortcut to setup64.exe, edit it to add option "--no-admin" on the command line.
Launch **setup64.exe** using the shortcut and choose "Install from internet";
Choose a mirror.
List of required packages:
(NB: to make "Install" appear, click once on "Default".
Otherwise, in order to see the detailed list of packages in a category, click on the "+" box left of the category name)

1. Vital Minimum
   (All : Default)
   Devel : make
2. Packages specific for compilation of OpenCALPHAD :

Search for "mingw64-x86_64" and click, in category "Devel", to select :

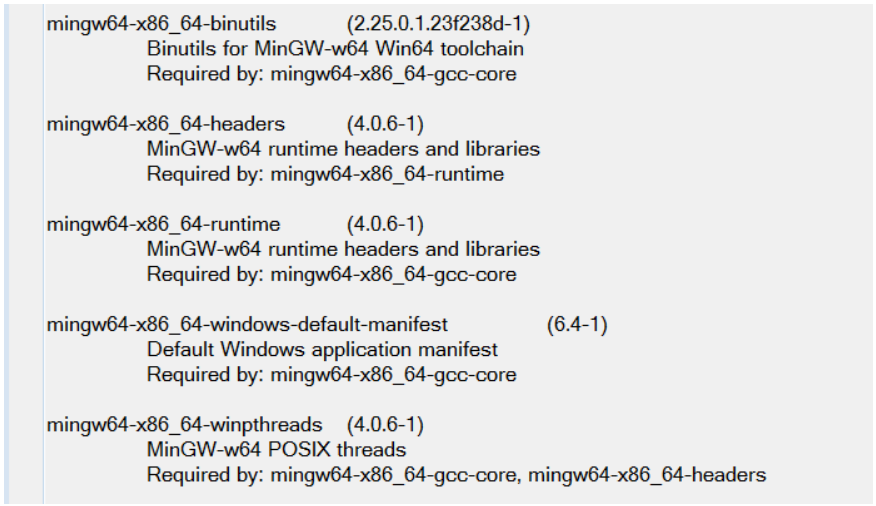


and



NB :

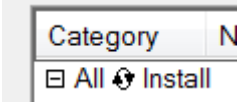
- *These choices will automatically trigger installation of the following dependencies :*



3. Optional but recommended : The following complementary packages add useful functionality such as opening local or distant graphical sessions
   (All : Default)
   Archive : bzip2, pax, unzip, zip, gzip
   Devel : git
   Editors : gedit, nano, nedit
   Graphics: gnuplot
   Web : wget
   X11: Install

4. Other packages

It is possible to complete this list in order to bring the system closer to a full linux system, but do not be greedy ! Never click to make



visible : the complete install takes at least 8 GB and 4 hours (as well as each update!). If you inadvertently did this, cancel installation and start again.

Follow up with installation without changing any default values (especially the installation folder).

Launching a cygwin command shell :
Start Menu / All programs / Cygwin / Cygwin terminal .

Launching the X server :
Start Menu / All programs / Cygwin-X : choose in the list any one of the X environments (e.g. XWin or WindowMaker or OpenBox or XLaunch or ...). NB : depending on which packages you installed, they may not all be functional.

Launching one or several (as many as you want) graphic terminals :
Start Menu / All programs / Cygwin-X / Xterm

2.3 Building parallel OpenCALPHAD within cygwin

Within a cygwin or xterm terminal enter the following commands :

```
cd /cygdrive/c/OPENCALPHAD     # adjust according to chosen install folder
cd opencalphad-version3        # adjust according to downloaded version
```

In order to run OpenCALPHAD under Windows it is necessary to build using a compiler whose name bears reference to "MinGW". Find your gfortran compiler in the list returned by the following command :

```
cygcheck -c -d | grep fortran | cut -d" " -f1 | xargs cygcheck -l {} | grep fortran.exe
```

If one of the "Makefile-*" files in the OpenCALPHAD distribution corresponds to your compiler copy it into a file named "Makefile" :

```
ls -l Makefile-*
cp  Makefile-x86_64-w64-mingw32  Makefile
```

Otherwise select the file whose name sounds closest (e.g. Makefile-parallel or Makefile-generic) and copy it into "Makefile" :

```
cp  Makefile-generic Makefile
```

and then edit this Makefile file with any text editor in order to adjust the compiler name.

It's ready for compilation. Enter the following command and carefully observe if it does not return error messages :

```
make
```

Launching and testing OC : see here.

3 Installing parallel OC under MSYS2

3.1 If MSYS2 is not present : installation

Install according to directions on https://msys2.github.io/ , giving particular attention to the following points (= problems) :

- Install under the user account that is currently active (as oppposed to : right-click and "launch as an Administrator"). Install for "Just for me" and not for "All users".
- According to item #9 in the procedure described on the website, browse to https://sourceforge.net/p/msys2/wiki/MSYS2%20installation/ in order to solve the problems. I ran into bug n° 4 :

"Sometimes a package upgrade fails with `failed to commit transaction (conflicting files)` and `some-pkg: /path/to/some/file exists in filesystem`. If you're sure you didn't put the offending files there manually, move or delete the files and start the upgrade again."

  - ⇨ Solution : Delete files "C:\msys64\mingw64.exe" et "C:\msys64\mingw32.exe" and redo the update steps.

3.2 Building parallel OpenCALPHAD under MSYS2

In a MSYS2 terminal (Start Menu / All programs / MSYS2 / MSYS2 MINGW 64-bits), enter the following commands :

```
cd /c/OPENCALPHAD              # adjust according to chosen install folder
cd opencalphad-version3        # adjust according to downloaded version
cp  Makefile-parallel Makefile
```

Enter the following command and check that it does not return error messages :

```
make
```

Launching and testing OC : see here.

4 Installing sequential OC under MinGW

NB : This may only be useful for users who already have an operational version of MinGW.

Start a Windows command terminal.

Check that gfortran is installed :
`gfortran --version`
The answer clearly shows if it's present or not.

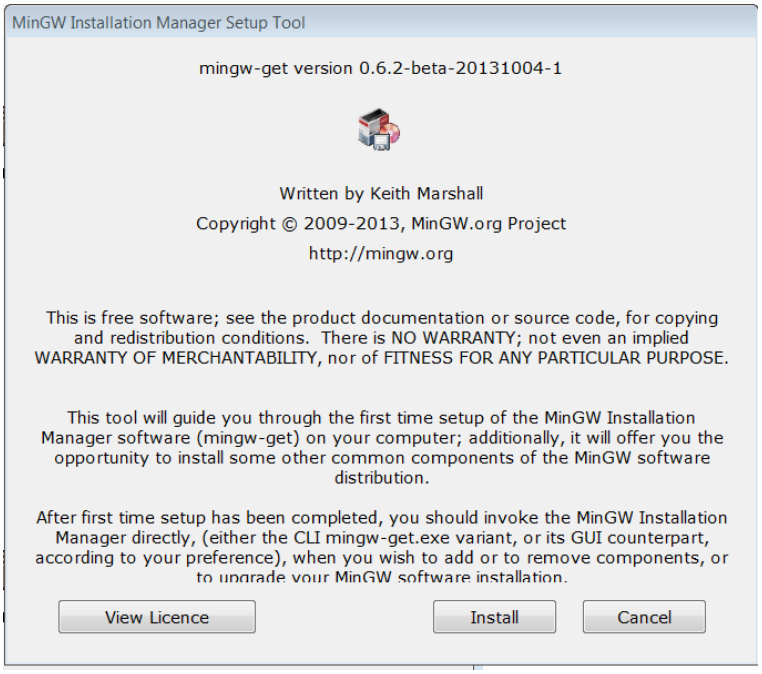
If gfortran is installed, go straight to building OC.
If not, then I warmly recommend to change your mind and pick another option : cygwin or MSYS2.
For those who persist in using MinGW, start by installing gfortran as described below.

4.1 Installing gfortran

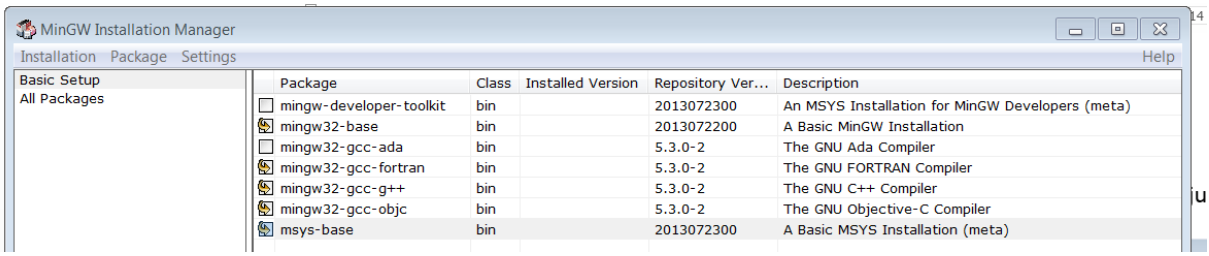
NB : really, I insist, nobody should be interested in this section.

See help on
http://www.mingw.org/wiki/HOWTO_Specify_the_Location_of_Libraries_for_use_with_MinGW
Note the last update of this help page (=2009). if you still want to install, do this.

1) Download MinGW gfortran 32 bits installer :
https://sourceforge.net/projects/mingw/files/latest/download?source=files



2) Launch it as a normal user (as opposed to admin), without changing anything until you reach the following dialog in which boxes should be checked as indicated here: (right-click and "mark for installation").



Start installation by clicking on "Installation / Apply changes"

3) Change PATH variable (see "modify environment variables" in Windows):
so that it includes (on the left)
c:\MinGW\bin;
Then OK.
Close the Windows session, open it agaain (so this variable is put in the environment).
In order to check that the new PATH is correct open a command shell (Start Menu / cmd) and enter :
gfortran --version
the answer should be e.g. "version 5.3.0".

4) In case of problems : delete the whole C:\MinGW folder and start again.

4.2 Installing opencalphad

Directions for this are given in the document "Installation\Install-OC-Windows-MinGW.pdf" of the OC distribution.

During the compilation step ("make"), check that "error" does not appear. In case the following message appears:

```
use omp_lib
      1
Fatal Error: Can't open module file 'omp_lib.mod' for reading at (1): No such file
or directory
```

search for all *.f90 source files (the list is given in the "linkmake" text file) that contain the offending "use OMP_LIB" or "use omp_lib" and comment those lines. Start again the compilation by entering :

```
make clean
make
```

Launching and testing OC : see here.

5 Launching and testing OpenCALPHAD

NB : binaries built using cygwin ou MSYS2 may also be launched from the Windows command shell.

5.1 Launching

The executable program is called "oc4A.exe" or "oc4P" ou "oc4P.exe" for version 4, it can be found in the root directory of the OC installation. To launch, open a terminal of your choice in the working directory and enter the command with its full path, such as :

- In a cygwin terminal :

```
~/OPENCALPHAD/opencalphad-version3/oc4P
```

- In an MSYS2 terminal :

```
/c/OPENCALPHAD/opencalphad-version3/oc4P
```

- In a Windows command shell :

```
C:\OPENCALPHAD\opencalphad-version3\oc4P
```

Open and read help files :

readme-general.pdf
OC3-commands.pdf
manual/ochelp3.pdf
documentation/*

5.2 Tests

Useful tests are provided as macros in the "macros/ocv4" folder. For example to try macro "map9", from the root directory of the OC installation :

```
cd macros/ocv4
../../oc4P
macro map9
```

Note in particular macro "`parallel2`" which is a benchmark for efficiency of parallelism and macro "`all`" which runs all macros in a row.

5.3 Adjusting the number of parallel processes

By default oc4P (and OpenMP in general) uses all the resources present on the computer : all cores and hyperthreading (if activated in the BIOS).

This behaviour can be changed by setting the environment variable **OMP_NUM_THREADS** which defines the maximum number of parallel processes that can be spawned by a given oc4P instance.

- Sous cygwin ou MSYS2 :

```
OMP_NUM_THREADS=1 ../../oc3P.exe
```

- Dans l'invite de commandes Windows

```
set OMP_NUM_THREADS=3
..\..\oc3P.exe
```

It may of course be set permanently by including it in the session environment initialization file.

6 Annex : installing GNUPLOT

First check whether gnuplot is installed. To do this, open a Windows command shell and enter :

```
gnuplot --version
```

The answer should be very clear.

6.1 In order to use OpenCALPHAD within the Windows cmd shell

Download one among the "gp*-win32-*" ou "gp*-win64-*" versions from :
(NB: ".exe" files require admin rights, "*.zip" files do not.)*
https://sourceforge.net/projects/gnuplot/files/gnuplot/

Install in a folder whose name does not contain any blank space character (e.g. C:\GNUPLOT).

If you chose the ZIP archive do not forget to adjust the PATH environment variable to include C:\GNUPLOT\bin.

6.2 In order to use OC within Cygwin

Building OC under cygwin as described in this document produces an OC binary that runs equally well within a cygwin terminal or a Windows terminal.

When it is launched from a cygwin terminal however, some configuration is needed so that the OC process be able to spawn the gnuplot process. In order to get htis behaviour :

- either inform cygwin of the path to the GNUPLOT installation under Windows by creating an alias such as (with possible path adjustment) :

```
alias gnuplot='cygstart /cygdrive/c/GNUPLOT/bin/gnuplot'
```

- or install `X11` and `gnuplot` packages within cygwin according to here.

7 Annex : The Windows command shell "cmd"

There are several ways to launch it.

(NB : This table remains to be proofread as I have no English version of Windows to check it!)

Method	**Folder location at start-up**
File explorer (Windows+E), open the desired working directory, "Uppercase+ right-click " in this folder, and select "Open a command shell here".	current working directory
"Start Menu" / All programs / Accessories / Command shell	HOME folder (according to environment variable)
"Start Menu" / enter "cmd " in the search box	
"Start Menu" / enter "cmd " in the search box	User profile root folder (C:\Users\toto)

8 Annex : "modify environment variables" in Windows

8.1 From within a cmd shell (and only for this shell session)

Use commands "`set`" et "`echo`".
Example to change the number of parallel processes :

```
set OMP_NUM_THREADS=3
echo %OMP_NUM_THREADS%
```

8.2 Permanently

"Start Menu" and enter "Modify environment variables" in the search box. Select "Modify environment variables for your account ". etc...