The Open Calphad Application Software Interface (OCASI)
Based on the TQ standard for interfacing thermodynamic software

Bo Sundman August 4, 2021

There is a Fortran version and a tentative iso-C version for C++. In the future it may be possible to merge these.

If you are not familiar with compiling and linking software and do not understand the intructions here please ask someone close to you for help. The instructions here are very brief but I am too busy to answer questions about handling such things and I know nothing about C++

To link any of the examples you must first compile and link the OC main program. When this works you must compile a special library excluding the file browser "tinyfiledialogs" and this is done (on Windiws) by the command file **makeocasilib**. You must first add the extension ".cmd" to this file and then execute it as a command/batch file. This generates the library files:

libocasi.a and **liboceqplus.mod**

Both of these files are needed to compile and link the applications.

The initial iso-C version of the library was provided by Teslos in 2014 and it has been extended by Matthias Stratmann at RUB, Germany and Christophe Sigli at Constellium, France to handle more calls to different subroutines. As things are still under development there may be slightly different versions on various subdirectories.

Files on this directory:

- readme.pdf is this file. There are specific readme files on the subdirectories.
- readme.tex is LaTeX source for this file. Subdirectories:
  - F90 has the source code for the TQ library, liboctq.F90 that was updated 1019.10.31 (Halloween) and three subqdirectories with examples.
    - The crfe/ was updated in October, 2019.
    - feni/ has not been upd ated for a long time.
    - parallel-alnipt/ simulating diffusion in Al-Ni-Pt in parallel added August 2021. There are instructions how to use it in the directory.
  - Cpp has one C++ example provided by Matthias Stratmann at RUB, Germany and one from Cristophe Sigli, Consillium, France. There is a separate version of the Fortran TQ library and an isoC interface. I tested the Scheil program in February 2020 and it works but it generates some error messages I do not

understand and as I do not know C++ I cannit fix that. I would be greateful for any help.

Note that STEP SCHEIL is now available as a command in OC.