The Open Calphad Application Software Interface (OCASI)

Based on the TQ standard for interfacing thermodynamic software

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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.

To link any of the examples you must first compile the OC main program. This compilation generates two files you need:

liboceq.a and liboceqplus.mod

Both of these files are needed for these 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 two subqdirectories with examples. The crfe/ was also updated in October, the feni/ I hope to update soon.
 - 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 am not able to update C++ code, anyone interested is wellcome to help.