Example using OCASI for a Scheil solidification simulation

Christophe Sigli and Bo Sundman February 24, 2020

Compiling and linking the example on Windows

- First run makeocasi in the installation directory to generate the files libocasi.a and liboceq-plus.mod
- Then come back to this directory
- Make linkscheil executable by: **copy linkscheil linkscheil.cmd**
- Execute linkscheil.cmd by: **linkscheil**
- This copies libocasi.a and some more files to this directory and compiles liboctq.F90 and liboctqisoc.F90 here and compiles them. At the end the command file links the program:

  g++ -o scheil -fopenmp -lstdc++ Example_OCASI.cpp liboctqisoc.o liboctq.o libocasi.a -lgfortran -lm
- Run the sample case by **scheil input.txt**

On the next pages the output generated is shown.

A run of the example on Windows

The program need an input file with commands, input.txt

The output below is captured from the screen, it generates the same output on the file output.txt and in a more condenced way on the file oc_log.txt

```
C:\Users\...\TQ4lib\Cpp\Scheil>scheil.exe input.txt
DEFINE_OUTPUT_FILE_NAME<output.txt>                  name of the log file

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                                    Open CalPhad Software Interface July 2016
                Computation performed on: 4 November 2016 , 22h:14mn:50s

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TDB_FILE_NAME<cost507r.tdb>          name of the thermodynamic data file

                                    TDB_FILE_NAME cost507r.tdb

 the following elements are in the database:
 AL / B / C / CE / CR / CU / FE / LI / MG / MN / N / ND / NI / SI / SN / TI / V
/ Y / ZN / ZR /
DEFINE_REF_ELEMENT<AL>
                                DEFINE_REF_ELEMENT AL
DEFINE_LIQUID_NAME<LIQUID>
                                DEFINE_LIQUID_NAME LIQUID
DEFINE_SOLSOL_NAME<FCC_A1>
                                DEFINE_SOLSOL_NAME FCC_A1
DEFINE_UNIT_COMPO_INPUT<W%>
                           DEFINE_UNIT_COMPO_INPUT W%
DEFINE_UNIT_TEMP_INPUT<C>                                        C or K
                            DEFINE_UNIT_TEMP_INPUT C
DEFINE_NCPU<8>
                                  DEFINE_NCPU 8
DEFINE_COMPOSITION<MG=5/SI=1>
                                DEFINE_COMPOSITION  tqini created: DEFAULT_EQUIL
IBRIUM
MG=5/SI=1
MG=5/SI=1
reading phases
 list of possible phases in the system :
```

```
 LIQUID AL12MG17 AL5FE4 ALCU_THETA ALLI ALMG_BETA ALMG_DZETA ALMG_UPSILON ALTI A
LTI3 BCC_A2 BCC_B2 BCT_A5
 CBCC_A12 CR3SI_A15 CRSI2 CUB_A13 DIAMOND_A4 FCC_A1 HCP_A3 LAVES_C15 MG24Y5 MG2S
I MGY_GAMMA SIV3
LIQUIDUS<>
                                          LIQUIDUS
* ----> liquidus is: 629.716 C

SOLIDUS<>
                                           SOLIDUS
* ----> solidus is: 587.599 C

COMPUTE_TRANSITION_TEMPERATURES<1100.0/400.0/0.0010000/20 >
                  COMPUTE_TRANSITION_TEMPERATURES 1100.0 / 400.0 / 0.0010000 /
20
first convergence issue
======================================================================
 TQ Parallel: Yes / number of threads: 8
 Here are the transition temperatures that have been found
 in the temperature range [400,1100] C
 for the following composition:
    0     629.72 LIQUID +
    1    629.715 LIQUID + FCC_A1
    2    592.104 LIQUID + FCC_A1 + MG2SI
    3    587.591 FCC_A1 + MG2SI

Store_Equilibria.size()=21
 elapsed time for the transition temperature routine (s)= 0.3205


COMPUTE_EQUILIBRIUM<500/3>
                                COMPUTE_EQUILIBRIUM 500 / 3

 Equilibrium at: 500 C fat%  FCC_A1=97.1874  MG2SI=2.81263
  MU(AL)= -28943.8
  MU(MG)= -47677.9
  MU(SI)= -44984.1
 ---------------------------------------
           FCC_A1
 ---------------------------------------
        AL =    96.5871 (W%)
        MG =     3.3932 (W%)
        SI =  0.0196668 (W%)
 ---------------------------------------
```

```
           MG2SI
 ---------------------------------------
        MG =    63.3809 (W%)
        SI =    36.6191 (W%)

LIQUIDUS<>
                                          LIQUIDUS
* ----> liquidus is: 629.716 C

SCHEIL_SOLIDIFICATION<castcompoS0001.txt/0.99500/1.0/0.1>
                            SCHEIL_SOLIDIFICATION castcompoS0001.txt / 0.99500
/ 1.0 / 0.1
first convergence issue
!!!!!!!! convergence issue !!!!!!!!!!!!!!!!!!!!
 Error setting condition:  T= 0.20000000E+04          2
Error code  4204 reset before calling grid minimizer
3Y Gridmin:     263 points   0.00E+00 s and       0 clockcycles, T=  722.87
Phases:   6 1 0.91 19 1 0.09 23 1 0.00
----------------------------------------
 starting composition in at :
AL = 0.935217 at
MG = 0.0552247 at
SI = 0.00955838 at
----------------------------------------
 concentrations left in FCC_A1 after Scheil solidification:
AL = 0.966794 at
MG = 0.0320182 at
SI = 0.00118751 at
----------------------------------------
 Phases formed after Scheil solidification:
fat(ALMG_BETA)=0.0203004
fat(FCC_A1)=0.954425
fat(MG2SI)=0.025275
----------------------------------------
========================================================================
 Here are the transition temperatures that have been found
     during a Scheil solidification simulation
    0    627.716 C  FL=  0.915013 LIQUID + FCC_A1
    1    590.716 C  FL=  0.300997 LIQUID + FCC_A1 + MG2SI
    2    449.716 C  FL=         0 ALMG_BETA + FCC_A1 + MG2SI
 end of solidification: 449.716

 elapsed time for the scheil solidification routine (s)= 0.640501
```

```
C:\Users\...\TQ4lib\Cpp\Scheil>
```