How to use map_mtdata_kinetics

1 Introduction

This program models the nucleation of growth of many phases in a parent matrix. The example application is that of precipitation in austenitic stainless steels. More details can be found in my thesis, available on http://www.msm.cam.ac.uk/phase-trans.
The program uses the MT-DATA (http://www.npl.co.uk/npl/cmmt/mtdata/mtdata.html) API interface.
The following provides step by step for the use of this program.

2 Compiling and installing

If you are reading this, you have uncompressed the archive file and hence have access to the *compile* script. You will need to edit it to point to the appropriate directory containing the MT-DATA object files.
Typically, this file should contain the lines:

```
f77 -c -w $1.f
echo " "
echo " *** Linking " $1.f
echo " "
f77 /path_to_object_files/*.o $1.o -o $2
```

To compile the program, type:

```
./compile kinetics kinetics
```

You can then run the executable file *kinetics*. Be sure that MT-DATA has permission to write in the directory from which you use the program.

3 Creating a .mpi file

3.a MT-DATA and .mpi files

When using MT-DATA on a system such as 'Fe,Cr,Ni,C', the user can either simply define the system and the sources (typically the SGTE solution and substance databases) in the MULTIPHASE module, then select the phases to work with. This is quick but the settings have to be repeated at each use.
Another method consists in first preparing a reduced dataset for the phases of interest (with the ACCESS module), then using it in MULTIPHASE. For example, instead of having to select a few of the 50+ phases found after a

define system 'Fe,Cr,Ni,C' source 'plus,sub_sgte' !

it is possible to use a file prepared with ACCESS which only contains the required phases:

define data 'mydata' !

3.b Creating a .mpi file

In this example, we create a .mpi file containing information for the phases FCC_A1, M23C6 and SIGMA. The following instructions also show the MTDATA prompt (all that is before ?).

```
WHICH MODULE ? access
ACCESS OPTION ? define system 'Fe,Cr,Ni,C' source 'plus,sub_sgte'!
ACCESS OPTION ? cla abs p(*) no p(FCC_A1,M23C6,SIGMA) !
ACCESS OPTION ? def out 'mydata' !
ACCESS OPTION ? save
ACCESS OPTION ? return
WHICH MODULE ?
```

At this point, we have a .mpi file called 'mydata' which we can use at any time in the MULTIPHASE module or, here, with the program.

4 Running kinetics

Be sure that the required files (spheregrowth.out, planargrowth.out, precipitate_data) are in the folder from which you run the program.
Lauch the program:

./kinetics

Enter the default for the power for time scale (0.5). This allows the time step to be increasingly larger as the precipitation progresses and transformation occurs on longer time-scale.
You are then presented with:

```
*************************************************************************
*                                                                       *
*****     CHOOSE BETWEEN:                                           *****
*                                                                       *
*         1) Use a global setting file                                  *
*         2) Create a global setting file                               *
*         3) Manual entry                                               *
*                                                                       *
*************************************************************************
```

Global files contains three informations: the mpi file to use, the composition file to use and the file containing information on the precipitates. They will considerably accelerate calculations repeated with similar parameters, but we are not yet able to create one as we have no composition files ready.

4.a Creating a composition file

In the above menu, select 3, you are presented with:

```
**************************************************************************
*                                                                        *
*****     MPI FILE:                                                  *****
*                                                                        *
*         To use this program, you should have prepared                  *
*         a mpi file with MT-DATA, using the ACCESS module.              *
*                                                                        *
*         WARNING: no more than 20 phases.                               *
*         What is the name of the file ?                                 *
*                                                                        *
**************************************************************************
```

Enter *mydata*, and you are presented with:

```
**************************************************************************
*                                                                        *
*****     Phases informations:                                       *****
*                                                                        *
*         This program requires information about the                    *
*         phases you will include in the calculation.                    *
*         They should be found in a file prepared with                   *
*         the program data.f                                             *
*                                                                        *
*         What is the name of this file ?                                *
*                                                                        *
**************************************************************************
```

Enter *precipitate_data* (this file is included in the package). You know see:

```
**************************************************************************
*                                                                        *
*****     Phases and information:                                    *****
*                                                                        *
*         FCC_A1     : missing:  nothing.                                *
*         M23C6      : missing:  nothing.                                *
*         SIGMA      : missing:  nothing.                                *
*                                                                        *
*         Enter whatever character to continue.                          *
*                                                                        *
**************************************************************************
```

The program is here displaying the status of the information it has on each phase found in the .mpi file. In this case, all informations required to perform a calculation with all phases have been found and the program indicates that nothing is missing.
WARNING although the program will indicate that some informations are missing on some phases, it will allow you to include such phases in a calculation, and generate meaningless results.
We now have:

```
**************************************************************************
*                                                                        *
*****     COMPOSITION AND TEMPERATURE                                *****
*                                                                        *
*         1) Use a file.                                                 *
*         2) Create a file.                                              *
*         3) Set manually.                                               *
*                                                                        *
**************************************************************************
```

Since we want to create a composition file, select **2**. You are successively asked to enter: the ageing temperature, whether your composition is in weight percent or mole percent, the mass of each component. Example here: 1023 (ageing temperature)
1 (in weight percent)
0.7 (Fe)
0.18 (Cr)
0.12 (Ni)
0.0003 (C)
You are then required to confirm your settings and select a file name, we can use *mydatac*. At this point, we have our composition file ready so we will abort (Control-C) to create a global file. You could however carry on with the simulation.

Restart *kinetics*, select 0.5 again for the time scale, then select **2) Create a global setting file**. You are presented with:

```
**************************************************************************
*                                                                        *
*****     ENTER SUCCESSIVELY:                                        *****
*                                                                        *
*         .the name of the mpi file                                      *
*         .the name of the data file                                     *
*         .the name of the composition/temperature file                  *
*                                                                        *
*         Enter END to go back to main menu                              *
*                                                                        *
**************************************************************************
```

Enter successively, according to our example:
mydata
precipitate_data
mydatac
then select a name for the global file, it can be identical to the .mpi file name since the former is stored without extension, so for example: mydata.
Again we could carry on here, but to illustrate the use of global files, we abort and restart.(Ctrl-C)
After restarting this time, select **1) Use a global setting file** and enter *mydata* as a file name. Everything going well, you are presented with two successive screens annoucing that no information is missing on the phases (as above), and that the composition file has been succesfully read. You then have:

```
**************************************************************************
*                                                                        *
*****     CHOOSE THE MATRIX AND THE PRECIPITATES                     *****
*                                                                        *
*                                                                        *
*         Although you can enter up to ten precipitates,                 *
*         only one is accounted for now, set it first.                   *
*                                                                        *
*         Enter the initial number of the phases for the                 *
*         matrix then the precipitates, 0 when finished.                 *
*                                                                        *
**************************************************************************

The phase FCC_A1              is normal
The phase M23C6               is normal
The phase SIGMA               is normal
```

By entering:
1
2
3
0
we actually select FCC_A1 as the matrix, M23C6 as precipitate 1 and SIGMA as precipitate 2.

4.b The solution treatment

We now reach the solution-treatment step. With austenitic stainless steels, a high-temperature (typically > 1200 °C) solution treatment is performed so as to dissolve as much precipitates as possible before service. However, part of the very stable phases such as TiC, NbC, TiN etc usually remains after the solution treatment. This step computes the equilibrium at high-temperature and set the composition of the matrix at this point as the new starting point.
In this case, we have to decide whether we want to include a solution treatment or not. Entering 0 will skip the solution treatment. We can however perform one, including all phases, and verify that they have been dissolved: Enter successively: 1, 2, 3 to include all phases. Then select 1473 for the temperature (always in K). If you scroll up, you should find the results:

```
 Moles and components mole fractions
-------------------------------------------------------------------
 FCC_A1          Fe          Cr          Ni          C
.180657E+02  0.6938157  0.1916234  0.1131783  0.0013826
-------------------------------------------------------------------

 New composition at the beginning of the ageing treatment:
 Fe:     69.979006298663
 Cr:     17.994601619035
 Ni:     11.996401079648
 C :     2.9991002653528D-02
```

which shows that indeed, only the matrix was found to be stable at this temperature.

4.c Diffusion coefficients

As we are working with austenitic stainless steels, we can use the coefficients calculated internally. When asked whether you want to enter some coefficients manually, answer **n**. We now have:

```
************************************************************************
*                                                                      *
*****     CHOOSING THE CONTROLLING COMPONENTS                    *****
*                                                                      *
*                                                                      *
*         How many controlling components for:                         *
*         M23C6                                                        *
*                                                                      *
*         Note that calculation time increase exponentially            *
*         with the number of controlling components.                   *
*         Enter 1 to use the bulk mass balance tie-line                *
*                                                                      *
************************************************************************
```

The number of controlling components is the number of components which control the growth rate of the precipitate. In theory, you could include all components here, but the calculation time would be far too long. In practice, include the main constituants of the precipitate. For example, Cr and C for M23C6. When components have similar diffusion coefficients, you can use a single controlling components, for example Cr for SIGMA.
Here we use two controlling components for M23C6 (Cr and C), and one for SIGMA (Cr). Enter **2**, you have now:

```
************************************************************************
*                                                                      *
*****     CHOOSING THE CONTROLLING COMPONENTS                    *****
*                                                                      *
*                                                                      *
*         Enter the active number in the list below:                   *
*                                                                      *
************************************************************************

     Active Component  1 is Fe
     Active Component  2 is Cr
     Active Component  3 is Ni
     Active Component  4 is C
```

We want component 2 and 4. Enter **2** and **4**. You are then presented with the same questions for SIGMA.
NOTE: If you select a component for which there is no diffusion coefficient, you will be asked to enter one.

We are nearly done. You now have to enter the wanted duration of the ageing treatment. We can select 100000 h, that is 3.6E8 s.

```
 Duration of the ageing treatment (s) ?
3.6e8
```

We then select the number of steps to be 5000. There can be significant error if the step is too large, however, as you increase the number of steps, you should observe convergence.

```
 Number of steps for the calculation ?
5000
```

Remains to give a name to the output file:

```
*************************************************************************
*                                                                       *
*****     Enter the name you want for the output file             *****
*                                                                       *
*                                                                       *
*************************************************************************
```

For the example, we can use **mydata_first**. Note that spaces are not allowed.
Displayed on the screen are the values of driving force, number of nuclei, local composition etc for each time step.

5 Controlling the output

The subroutine snapshot can be easily edited to obtain output of most of the variables evaluated during the calculation:

```
C ***********************************************************************
C
C subroutine snapshot: here all the common variables are declared and
C it is easy to modify the output to a file. By default, the total volume
C transformed, the nucleation rate and the driving force will be written
C to a file as a function of time.


      SUBROUTINE SNAPSHOT(TIM)

...

      WRITE(2,100) TIM,RADII(1,1,1),(VFRAC(PCP),PCP=1,10)
```

For example, configured as above, the output contains the radius of the precipitate 1 (M23C6 in our example), for the precipitate nucleated at t=0, and the volume fractions of all precipitates.