commented run of DOMINO

P-T equilibrium assemblage diagram

We will calculate a P-T equilibrium assemblage diagram for Temperatures between 500 and 900 ^{o}C and Pressures from 1 to 13 KBar.
This example uses the database JUN92.bs. The bulk composition corresponds to 10 paragonite and 10 muscovite, with excess H_2O and SiO_2.
Edit the dat-file (usually called THERIN of therin.txt) file, so that the first two lines (not counting the comment lines beginning with "!") are as follows:

```
600     4000
1   SI(160)AL(60)NA(10)K(10)H(100)O(?)     *
```

Start the program DOMINO: In a UNIX shell or in the Mac OsX Terminal or in the "start.bat" batch window on a PC you type the command "domino" and enter Return.

In the following, the framed text (font courier) is the screen output of the program.
The bold text (font courier) is the user input (typed in the keyboard)

domino

```
Program DOMINO, Version (dd.mm.yy) 01.08.09 (MacOsX, gfortran)
 ============================================================

 "Computation of phase diagrams in complex systems"


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 ================================================================================
```

This is the prolog of the program. Depending on the version used and the platform, the first few lines may look slightly different or may be missing. Some lines may have been inserted by the person installing the program as a control, that the correct directories were chosen. (or to add their own name as author).
The title includes the version number, the operating system and the compiler used to install the software.

```
--------------
 initialization
 --------------
 Initialization-file:   /user_capi/capi/gnugnu/DominoTheriak111207/theriak.ini
 Program's directory:   /user_capi/capi/gnugnu/DominoTheriak111207/
 Working directory:     /user_capi/capi/gnugnu/tests_and_examples/pixelmapsandH2Oact/

 Run: 16.06.2009 - 22:18:02
```

Program's directory: Depending on the installation and how you invoke the program, this is the absolute or relative path of the directory containing the running program.

Working directory: Current directory from where you typed the command. (**However**: if this directory does not contain a dat-file (containing P, T and bulk composition) the working directory will be set equal to the program's directory.

In order to run, the program needs the initialization file "theriak.ini". (This file contains the personal settings, like calculation parameters and the file names of input and output). If "theriak.ini" is found in the working directory, this will be used. If not, the one in the program's directory is used. In neither is found, the program stops.

The run is identified by the date and time.

```
------------------
 database definition
 ------------------
 Enter [ "?" | CR | "files" | "script" | database filename ] < >?
```

At this point the program asks for a database file. If a log-file (a file containing most interactive input from a previous run) exists, the last used database filename is proposed, which you can accept by entering an empty line (CR). Else you type the file name of the database, which must be located in the working directory.

The keyword "files" will provide you with the information on file names as defined in "theriak.ini"

The keyword "script" is used to define several domino-runs, which are to be run as batch-job.

JUN92.bs

```
--------------------
 definition of X-axis
 --------------------

 X-variable may be: TC, TK, P, A(abc), LNA(abc), LOGA(abc), BIN, TER

 Enter [ "?" | "list" | CR | X-variable  X-min  X-max  (X-Grid)  (width)] < >?
```

Define the X-axis: (Note that you have to enter at least **two blanks** between items)
We choose TC (which is the Temperature in ^{o}C) with a lower limit of 400 and an upper limit of 900 ^{o}C.
The initial grid for DOMINO (xGrid) is 10 and the width of the Diagram (width) is 15 cm (default values).

TC 500 900

```
--------------------
 definition of Y-axis
 --------------------

 Y-variable may be: TC, TK, P, PT, A(aBc), LNA(aBc), LOGA(aBc), BIN

 Enter [ "?" | CR | "list" | Y-variable  Y-min  Y-max  (Y-Grid)  (height)] < >?
```

Define the Y-axis: (Note that you have to enter at least **two blanks** between items)
We choose P (which is the Pressure in Bar) with a lower limit of 1 and an upper limit of 10000 Bar.
The lower limit cannot be given as "0", because the program only accepts positive pressures. If desired, the labeling and the dimensions of the axis may be edited in the graphics output file.
The initial grid for DOMINO (y-Grid) is 10 and the width of the Diagram (y-Dim) is 15 cm (default values).

P 1000 13000

```
------------------------------
 definition of calculation type
 ------------------------------

 to calculate                          enter
 ------------                          -----
 equilibrium phase diagram              "." (dot)
 isolines:
    special funtions:                          Key      min  max  step
    non-solution phases:                Name   Key      min  max  step
    solution phases:                    Name   Key  Nr  min  max  step

 For help with isoline definition type "i".


 Enter [  "?"  |  CR | "list" | "i" | "." |
       | "pix" ix iy | (Phase)  Key  (Nr)  min  max  step ] < >
```

The user input is "." (a dot). This means we calculate an equilibrium assemblage diagram.

•

```
---------------------
 labeling of reactions
 ---------------------

 Labels: 1=assemblages, 2=new phases, 3=reactions, -1=special

 Enter [ "?" | CR | Label (prec  smooth) ] < >?
```

It is strongly recommended to use label=1. Thus all "reactions" are labeled on each side with the abbreviations of all phases present. (label=2 makes shorter labels, omitting all phases present on both sides, and label=3 works only for simple systems with no continuous reactions.)
The precision and smoothness (prec smooth) are left at their default values of 0.005 and 0.04. The precision defines how many levels of refinement are necessary for the diagram.

1

```
 X: Temperature [C]
 Y: Pressure [Bar]
 MAXIMUM LEVEL:   6  PREC = 0.0050  WPREC = 0.0400
```

The above output is a short summary, with the axis labels, the maximum level of refinement, the precision and the smoothness (here called WPREC)

Now computation starts.

```
ASSEMBLAGE:   1: x,y =  5.00000E+02   1.00000E+03  FSP WHITE MICA aQz And H2O
      assemblage: FSP_Ab WHITE_MICA_Ms aQz And H2O
 ASSEMBLAGE:   2: x,y =  5.80000E+02   1.00000E+03  (2)FSP aQz And H2O
      assemblage: FSP_Ab FSP_Kfs aQz And H2O
 ASSEMBLAGE:   3: x,y =  6.20000E+02   1.00000E+03  (2)FSP bQz And H2O
      assemblage: FSP_Ab FSP_Kfs bQz And H2O
 ASSEMBLAGE:   4: x,y =  6.60000E+02   1.00000E+03  FSP bQz And H2O
      assemblage: FSP_Ab bQz And H2O
 ASSEMBLAGE:   5: x,y =  7.00000E+02   1.00000E+03  FSP bQz Si H2O
      assemblage: FSP_Ab bQz Si H2O
 REACTION:  1   1  =   2
 LABELED WITH ASSEMBLAGES
 REACTION: FSP WHITE MICA aQz And H2O = (2)FSP aQz And H2O
 REACTION:  2   2  =   3
 LABELED WITH ASSEMBLAGES
 REACTION: (2)FSP aQz And H2O = (2)FSP bQz And H2O
 REACTION:  3   3  =   4
 LABELED WITH ASSEMBLAGES
 REACTION: (2)FSP bQz And H2O = FSP bQz And H2O
 REACTION:  4   4  =   5
 LABELED WITH ASSEMBLAGES
 REACTION: FSP bQz And H2O = FSP bQz Si H2O
     47    47  Y =  1000.0000 ,      4 REACTIONS:    1    2    3    4
...
```

The program starts with scanning along the initial grid for assemblages and reactions.

Each time a new assemblage is found a comment is printed, e.g.:

```
 ASSEMBLAGE:   1: (2)FSP aQz And H2O
 ASSEMBLAGE:   2: (2)FSP bQz And H2O
```

Assemblage Nr.1 is: two feldspars, α-quartz, andalusite and water.
Assemblage Nr.2 is: two feldspars, β-quartz, andalusite and water.

The border between two assemblages is defined as "reaction":

```
 REACTION:  1   1  =   2
```

Reaction Nr.1 is the border between assemblage Nr.1 and assemblage Nr.2.

When one grid-line is scanned the comment is e.g.:

```
      47    47  Y =    1.0000 ,      4 REACTIONS:  1  2  3  4
```

The first number (47) is the count of equilibrium calculations for this grid-line; the second number (also 47) is the total of equilibrium calculations so far. The grid-line is along the x-axis at y=1 (=1 Bar). Four reactions were found, namely reactions Nr.1, Nr.2, Nr.3 and Nr4.

etc. etc.

```
...
23   816  X =   820.0000 ,      3 REACTIONS:   19   18   17
     18   834  X =   860.0000 ,      2 REACTIONS:   19   18
      9   843  X =   900.0000 ,      1 REACTIONS:   19
 NUMBER OF LINES:  22    NUMBER OF POINTS:  86    max.ph.   67
...
```

Eventually the grid-lines are all scanned and refinement begins. At this point (and after each level of refinement), a rough phase diagram (now containing only points that lie on the initial grid-lines) is saved to the graphics output file. The program may be interrupted and a rough diagram plotted. In this example the diagram consists of 21 lines with a total of 85 points.

At each level, each line is checked for smoothness (BUMP), open ends (OPEN END) or too few points (TWO POINTS). If the line needs refinement, the grid is halved in the vicinity of the line and searched for new reaction-points:

```
...
LEVEL:  0   SQUARE: (  3 ,  1 ) LINE     2   REACTION    2: OPEN END
     11   881  Y =  1600.0000 ,      1 REACTIONS:    2
     10   891  X =   600.0000 ,      1 REACTIONS:    2
 NUMBER OF LINES:  22    NUMBER OF POINTS:  91    max.ph.   53
...
```

Comments:
- At level "0" (initial grid) line Nr.1 (labeled as reaction Nr.1) has an open end in the mesh (x=5, y=2)
- After 19 equilibrium calculations (adding to a total of 869) along the x-axis at y=1500.85 (Bar) two new points are found: one for reaction Nr. 1 and one for reaction Nr. 21.
- After 10 equilibrium calculations (adding to a total of 879) along the y-axis at y=625 (^{o}C) one new point is found for reaction Nr. 21.
- Now the diagram consists of 21 lines with 88 points.

etc. etc.

After refining for five levels, the necessary precision is reached and the calculation stops:

```
...
REACTION: 26  13  =   5
 LABELED WITH ASSEMBLAGES
 REACTION: FSP aQz Ky H2O = FSP bQz Si H2O
      6  2154  Y = 10431.2500 ,      1 REACTIONS:   26
      7  2161  X =   816.8750 ,      2 REACTIONS:   19   18
 NUMBER OF LINES:  26    NUMBER OF POINTS: 276    max.ph.   66

exit DOMINO
CPU time:    0h 00m 08.71s
```

The diagram now consists of 26 lines with 276 points.
The graphics file for the equilibrium assemblage diagram is written (in this example) to the file "coplot".

Running GUZZLER

The labels of the reactions in the graphics file are not yet visible (size =0). The program GUZZLER assigns a size and distributes the labels. Four cases are distinguished:

1) Full label is written
2) Only the number of the label is written on the curve.
3) The number is written somewhere close, with a fine line pointing to the reaction.
4) The curve is not labeled at all

Like all software that appears to do some "thinking", GUZZLER is quite straight forward and does not do any thinking at all.

Start the program GUZZLER. Enter the command "guzzler".

guzzler

```
Program (THERDOM):   /user_capi/capi/gnugnu/DominoTheriak111207/

 path for program:    /user_capi/capi/gnugnu/DominoTheriak111207/

 Working directory: /user_capi/capi/gnugnu/tests_and_examples/pixelmapsandH2Oact/


Program GUZZLER, Version (dd.mm.yy) 01.08.09 (MacOsX, gfortran)
================================================================

"Labeling reactions in graphics files"

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================================================================================
RUN: 16.06.2009 - 22:31:07

try working directory: /user_capi/capi/gnugnu/tests_and_examples/pixelmapsandH2Oact/guzzler.last

log-file used: /user_capi/capi/gnugnu/tests_and_examples/pixelmapsandH2Oact/guzzler.last
```

Depending on the version used and the platform, the first few lines may look slightly different or may be missing.

```
Enter [ "?" | CR | graphics file name ] <coplot>?
```

"coplot" is the name of the graphics file written by DOMINO. (in this example).

coplot

```
working directory: /Volumes/user_capi/capi/gnugnu/newdemos/

Enter [ "?" | CR | size of labels ] <0.2>?
```

The comment on the working directory is for testing purposes.
Even with no log-file present, the program will propose 0.2 for the size of labels (in cm).

<CR> (return)

```
1):  FSP WHITE MICA aQz And H2O = (2)FSP aQz And H2O
   2):  (2)FSP aQz And H2O = (2)FSP bQz And H2O
   3):  (2)FSP bQz And H2O = FSP bQz And H2O
   4):  FSP bQz And H2O = FSP bQz Si H2O
   5):  (2)WHITE MICA aQz H2O = WHITE MICA aQz H2O
   6):  WHITE MICA aQz H2O = FSP WHITE MICA aQz And H2O
   7):  (2)FSP aQz And H2O = (2)FSP aQz Si H2O
   8):  (2)FSP aQz Si H2O = (2)FSP bQz Si H2O
   9):  (2)FSP bQz Si H2O = FSP bQz Si H2O
  10):  WHITE MICA aQz H2O = FSP WHITE MICA aQz Si H2O
  11):  FSP WHITE MICA aQz Si H2O = (2)FSP aQz Si H2O
  12):  (2)WHITE MICA aQz H2O = FSP WHITE MICA aQz Ky H2O
  13):  FSP WHITE MICA aQz Ky H2O = FSP WHITE MICA aQz Si H2O
  14):  (2)FSP aQz Si H2O = FSP aQz Si H2O
  15):  FSP aQz Si H2O = FSP bQz Si H2O
  16):  FSP WHITE MICA aQz Si H2O = FSP aQz Si H2O
  17):  FSP WHITE MICA aQz Ky H2O = FSP aQz Ky H2O
  18):  FSP aQz Ky H2O = FSP bQz Ky H2O
  19):  FSP bQz Ky H2O = FSP bQz Si H2O
  20):  (2)WHITE MICA aQz H2O = FSP WHITE MICA aQz And H2O
  21):  FSP WHITE MICA aQz Si H2O = FSP WHITE MICA aQz And H2O
  22):  (2)FSP bQz Si H2O = (2)FSP bQz And H2O
  23):  (2)WHITE MICA aQz H2O = FSP WHITE MICA aQz Si H2O
  24):  FSP aQz Ky H2O = FSP aQz Si H2O
  25):  (2)FSP aQz Si H2O = (2)FSP bQz And H2O
  26):  FSP aQz Ky H2O = FSP bQz Si H2O
```

A numbered list of all reactions is printed. The same list ist also written to the rxn-file (in this case called "table")

```
--------------------------------------------------------------------------------
 Most important options for labeling:
  -3: automatic (default)      0: no labels or numbers      5: no offset numbers

 Enter [ "?" | CR | option  (min_length)] <-3  0.020>
```

At this point the user coud have some influence on labeling. (E.g. for a clean diagram with no labels choose the option "0".)

<CR> (return)

```
25): NO LABEL
  26): NO LABEL

exit GUZZLER
```

All reactions which could not be labeled are listed. These are usually very short line segments or single points.

The cleand-up graphics file is written to the cln-file (in this example it is called "clean")

Running EXPLOT

This program translates the graphic file into a PostScript file.

Start the program EXPLOT. Enter the command "explot".

explot

```
Program (THERDOM):   /user_capi/capi/gnugnu/DominoTheriak111207/

 path for program:    /user_capi/capi/gnugnu/DominoTheriak111207/

 Working directory: /user_capi/capi/gnugnu/tests_and_examples/pixelmapsandH2Oact/


Program EXPLOT, Version (dd.mm.yy) 01.08.09 (MacOsX, gfortran)
================================================================

"Create a PostScritp(TM) file from graphics input"

Written by:
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Input dialogue and help by:
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          E-mail: konstantin.petrakakis@univie.ac.at

================================================================================
Run: 16.06.2009 - 22:36:23


log-file used: /user_capi/capi/gnugnu/tests_and_examples/pixelmapsandH2Oact/explot.last


Enter [ "?" | graphics file name ] < >?
```

"clean" is the graphics file written by GUZZLER. There is no further input.

clean

```
working directory: /user_capi/capi/gnugnu/tests_and_examples/pixelmapsandH2Oact/

exit EXPLOT
```

The output of EXPLOT is a PostScript file (pst-file), which in this case is called "plot.ps". (Some platforms recognize the ending ".ps" and the appropriate program will open it.)
The PostScript file may be viewed (and even modified) by several programs, e.g. Adobe Illustrator, Corel Draw, PreView or ghostview (UNIX).

The following image is made from Adobe Illustrator with no further editing:

Calculated equilibrium phase diagram