How to get started with Theriak-Domino
and some Worked Examples

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If you can follow instructions, you can download and install Theriak-Domino. However, there are several folders and many files in the download packet, and sorting it all out can cause some confusion. So, below are suggestions for a way to proceed. These instructions are really just streamlined versions of what is in the Theriak-Domino Users Guide that you can download with other program files from Christian de Capitani's Theriak-Domino website.

These instructions are current as of June 20, 2011, when I downloaded Theriak-Domino to make sure I had the most recent versions of everything. If a new version is put on the download site, things might change a bit. Note: what follows applies specifically to Windows users but Mac users may wish to figure out how to do the same thing.

Besides these instructions, be sure to check out the users guide's that come with Theriak-Domino.

Setting it Up (instructions current as of June 20, 2011)

1. Go to http://titan.minpet.unibas.ch/minpet/theriak/theruser.html
    This will get you to a main Theriak-Domino page with some very useful information.

2. Decide what root folder you are going to use for all the Theriak-Domino files and folders. It can be anything. I use a folder called *TD* for this purpose in the instructions that follow, but you could substitute something else (*e.g.*, *Programs/Theriak-Domino* or simply *Theriak-Domino)*. Or, you can stick with the folder name you will get after you download and unzip the program package (which was *TheriakDominoWIN* when I downloaded the files on June 20, 2011). If you choose to change the root folder, make the change where *TD* appears below in these instructions.

3. Click on the appropriate link to the download page and follow instructions there. After unzipping (usually accomplished by double clicking on the zip-file folder name) put all files and folders in your root folder. You should have four subfolders in your root folder:
• 	*Documentation* – contains most importantly the *TheriakDominoGuide.pdf*. This guide has installation instructions and much other necessary information that you will need at some point.
• 	*Examples* - This folder contains what you expect.
• 	*Programs -* This contains both compiled and source versions of programs and some important support files.
• 	*Working* - Whenever you want to do calculations, you will start in this folder.

The *Working* folder contains the different thermodynamic databases.

The *Working* folder also is where you will create input data files for calculations and where output files will accumulate.

The *Programs* subfolder contains all the compiled programs. (You may never have to look at the contents of this folder again once you have the programs installed and running.)

For routine calculations, only *theriak.exe* and *domino.exe*, *guzzler.exe* and *explot.exe* are used.

**NOTE: If you cannot see the suffixes on file names (file extensions such as *.exe*, *.txt*, etc.) when you look at a file directory, you may be well served to make them visible. In Windows 7, go to start>control panel>folder options>view and uncheck "hide extensions for known file types." In other versions of Windows the instructions are not quite the same.

Editing Data/Control Files

4. You need to (a) tell Theriak-Domino where the program files are stored on your computer. Additionally, to make

editing and copying results easier and more straightforward, it is best that (b) input files be *.txt* files, and (c) copies of the calculation results be written to *.txt* files. Also, to avoid confusion, it is best (d) to eliminate files of the same name that appear in more than one folder.

So, go to the *Working* folder and:

a. Make sure it contains a file called *start.bat*. (If not, there is probably a *.bat* file with a different name that is essentially the same.) Right-click on *start.bat* and edit the file so that it includes these three lines:
> set THERDOM=c:\TD\Programs\
> set PATH=%THERDOM%;%path%
> cmd

By setting the path, you are telling Theriak-Domino where the program files are stored. So, If your root folder for Theriak-Domino is not *TD*, put in the correct folder name instead of *TD*.

b. Make sure there is a file in the *Working* folder called *therin.txt*. If there is also one called *therin* (with no suffix) rename it as *xtherein* (by putting an "x" in front of the name) so there is no confusion later. (Or, you can delete it, but I worry about deleting files that maybe, just maybe, I might need.)

Now, go to the *Programs* folder:

c. Edit the file called *theriak.ini* (*Programs* folder) as follows: scroll down to the section near the bottom called *"Program-files blocks,"* and change the first two blocks to contain what is in the box below. (Changed lines are in bold italics below):

```
$THERIAK-FILES
dat=therin.txt          #User's chemical input to program
dbs=Run-time-defined    #Thermodynamic data base to be used
log=theriak.last        #User's responses during last run of program
out=thkout.txt          #Calculation information to be printed or viewed on screen
bin=binout              #Graphics data for "pseudo-binary system" calculations
drv=Run-time-defined    #"Special calculation" directives for running the program
tab=loop_table          #Table of variable values; input to a spreadsheet program
tcp=loop_tecplt         #Table of variable values; input to "TechPlot"
inf=loop_info           #info for Table of variable values
$END


$DOMINO-FILES
dat=therin.txt          #User's chemical input to program
dbs=Run time-defined    #Thermodynamic data base to be used
log=domino.last         #User's responses during last run of program
out=domout.txt          #Calculation information to be printed or viewed on screen
plt=coplot              #Graphics data (e.g., input to GUZZLER)
cln=clean               #Graphics data after label arranging and cleaning (e.g., input to EXPLOT)
pst=plot.ps             #Graphics file in PostScript format
fig=pixelmaps           #Directory name for pixelmaps (no filename extension!)
$END
```

d. In the Programs folder, you may find redundant files called *therin* or *therin.txt*. I suggest you rename them by putting an "x" in front of their names so that the only copy is *therin.txt* in the *Working* folder. This means your students (or you?) won't edit the wrong file later and wonder why the changes did nothing!

Take special care as you do steps a, b, c, and d, above. No typos, please.

<u>**Setting Up the DOS Console Window**</u>

5. **Optional but highly recommended:** All calculations are done in a DOS command console window. To see as much output as possible without scrolling, and to avoid having output scroll away and disappear, you should adjust the default size of the console window.

   Go to the *Working* folder and double click on *start.bat*.
   The console widow will open. Right click on the console title bar and select *properties*.
   Click the *Layout* tab.
   Adjust the *screen buffer size* to a width of 133 (or something else depending on your monitor size) and a height of at least 200.
   Also physically adjust the window size on your monitor (by dragging handles) depending on your monitor size. Typically I have the console window cover about 75% of my monitor.
   And, if you wish to change the console background color or font, click on *properties>colors* and change as you wish.
   When done with all adjustments, click on *OK*.

<u>**Is it Working?**</u>

To see if your have things set up correctly for Theriak:
- Go to the *Working* directory
- Double click on *start.bat*
- At the console prompt, type   *theriak*
- It will request the name of a database. Respond: *jun92.bs*
- It will ask you about the type of calculation. Respond: *no*

Theriak should run to completion with no error messages.

To see if your have things set up correctly for Domino:
- Go to the *Working* directory
- Double click on *start.bat*
- At the console prompt, type   *domino*
- It will request the name of a database. Respond: *jun92.bs*
- It will ask what is on the X-axis? Respond: *tc 600 1000* ←note: you must have <u>2</u> spaces
- It will ask what is on the Y-axis? Respond: *p 1000 10000*   after tc, 600, p and 1000
- It will ask about the calculation type. Respond: *.*   ←note: response is a period
- It will ask about labels. Respond: *1*

Domino should run to completion with no error messages.

Hints and Notes about doing Theriak-Domino Calculations

- **Domino**'s main purpose is to calculate and plot equilibrium phase diagrams.
- **Theriak**'s main purpose is to calculate stable mineral assemblages and compositions.
- The other programs, except for the plotting programs, may not be of interest to you.

- All calculations are carried out in a DOS console window that is invoked by double clicking *start.bat*.
- After invoking *start.bat* a program is started by typing its name (*e.g.*, **Theriak**) at the console prompt, followed by CR.
- Some programs are chained – output from one becomes input for another.
- All input and output data should be in text (*.txt*) files so they are easily opened and edited. These files will probably open in *Notepad* if you double click their names in the folder directory – making editing easy.
- You can have more than one *Working* folder if you want to keep projects separate.

- The file *therin.txt* is the input file for Domino and Theriak calculations. It makes it much easier to read and edit this file if it is small. But, when you first download it, it may contain mostly comments (lines that begin with an exclamation point). Delete all the comments after you figure out what is going on. Also, only one line of chemical data is used, unless you are calculating binary or ternary diagrams, so delete all except the first line of chemical data if there is more than one. For most calculations, *therin.txt* will only contain two lines, something like this:

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

- When doing calculations you will often find yourself going back and forth between the *Working* folder, the *Notepad* editor, and the *console* window. The best way to do this is to have them all open on the desktop, overlapping and piled on top of each other so you can click from one to the other easily.

Defaults when entering values

After you have run a program once, it will remember what you responded to prompts the previous time and that becomes a default answer. Your last response will appear between < and > at the end of each prompt. So, if you like that answer you only need to hit enter -- there is no need to type anything else. If you don't like the default, type whatever you wish and hit enter. Example:

The first time you run Theriak, it will prompt you with

Enter ["?" : CR : "files" : database filename]?

If you enter *jun92.bs*, the next time you run the program, the prompt will appear as

Enter ["?" : CR : "files" : database filename] <*jun92.bs*>?

and you need only hit enter to accept the default.

Doing Calculations

■To do a standard Theriak calculation you will:

- Edit *therin.txt* so it contains the correct T, P, and composition.
- Navigate to the *Working* folder, then double click on *start.bat* to get to the DOS console.
- Type "theriak" and hit enter.
- Type in the name of the thermodynamic database and hit enter (or accept the default by just hitting enter).
- Respond "no" to the next question if you just want to do a standard calculation.

The program will then run and print out lots of results. (The amount of output depends on information in *therin.txt*). A copy of the output will be in the file *thkout.txt*.

■To do a standard Domino calculation you will run Domino, followed by Guzzler, followed by Explot:

Domino
- Edit *therin.txt* so it contains the correct T, P, and composition.
- Navigate to the *Working* folder, then double click on *start.bat* to get to the DOS console.
- Type "domino" and hit enter.
- Type in the name of the thermodynamic database and hit enter (or accept the default by just hitting enter).
- Enter the temperature range and hit enter (or accept the default by just hitting enter).
- Enter the pressure range and hit enter (or accept the default by just hitting enter).
- Type a period followed by enter for a standard calculation (or accept the default by just hitting enter).
- Type 1 and hit enter to have assemblages listed on output (or accept the default by just hitting enter).

The program will run and print out results that may be meaningless until you become familiar with how Domino works. Domino will also create a file called *coplot* which is used in the next step. When Domino is done you will be back at the console prompt. The file *domout.txt* will contain the same output that scrolled on the screen during calculations.

Depending on the number of components and phases, Domino takes a few seconds to several 10's of minutes to execute.

Guzzler
Now run Guzzler to clean up the plot data:
- Type "guzzler" and hit enter to clean up the plot output.
- Respond **coplot** and hit enter when it asks where the graphics input file is (or accept the default by just hitting enter).
- Respond **0.2** and hit enter to tell it the size of font to use (or accept the default by just hitting enter).
- Just hit enter when asked about other options.

Guzzler will then run, print out some results, and return you to the console prompt. It will create the file *clean* which is used in the next step. *Guzzler takes very little time to execute.* Guzzler puts a list of all reactions in the file called *table*.

Explot
Now run Explot to create a diagram:
- Type explot and hit enter.
- Type *clean* to tell it the graphics plot name (or accept the default by just hitting enter).

Explot will then run and return you to the console prompt. Your graphics output is now in a postscript file called *plot.ps*. *Explot takes very little time to execute.*

To see your results, in the *Working* folder directory, double click on *plot.ps* and it will open in whatever your computer has set for the default to view postscript files. A list of all reactions is in the file *table*.

Example Calculations

Example Calculation #1 (Theriak calculation a single T and P)

1. Go to the *working* folder and open *therin.txt*. Edit and save it so that it contains these two lines:
   700 3000
   0 NA(0.5)K(0.5)AL(1.0)SI(3.0)O(8.0)SI(10)O(20)H(20)O(10) *

   (Note: elemental symbols <u>must be in all caps</u> – easy to forget, and if you do forget the program will produce a "fatal error.")

   This is a typical input for a simple equilibrium calculation. The temperature is 700 °C, the Pressure 3000 bar. The bulk composition (numbers are moles) corresponds to 0.5 K-Feldspar + 0.5 Albite, with "excess" (10 mole) SiO2 and H2O. The 0 at the beginning of the second line produces a short output (only the basic results) and the star "*" at the end means, that all matching phases in the database are to be considered.

2. Start Theriak and enter the following responses (**that are in bold**) to the prompts:
   database   *jun92.bs*   <= *you are selecting the jun92.bs database*
   type of calculation   **no**   <= *this is NOT a special kind of calculation*

   The program will then do its calculations. The results, which may seem a bit arcane until you get used to them, will tell you that for the composition you entered, at 700 °C and 3000 bar, the equilibrium assemblage will contain 1 mole of feldspar that is 50-50 albite-K-feldspar, 10 moles of quartz, and 10 moles of H2O vapor.

   This was a simple calculation at a single PT. You can, if you wish, have the program do calculations at multiple TPs or in a loop, say for example from 500 to 1000°C at 100° intervals. See Example Calculation #2.

   *The output from Theriak that you saw on the screen is also in the file *thkout.txt* – making it easy to grab values and put them in a spread sheet or whatever else you want to do.

Example Calculations #2 (Theriak calculations at multiple Ts and Ps)

Example 1 gets you output for 700 °C and 3000 bar. Suppose you want output at several different PT conditions? There are two basic ways to do this.

Method #1. Change the type of calculation to **"loop"** – instead of **"no"** when prompted, otherwise do the calculation as you did for *Example #1*. The program will ask you for a P and T, do a calculation, ask you for another P and T, do another calculation . . . and keep going until you just enter nothing followed by a CR.

Method #2. Suppose you want to calculate equilibrium assemblages along a TP path at fixed intervals. For this example, assume you want calculations from 750° to 1000° at 3000 bars.

1. Go to the *Working* folder and open *therin.txt*. Edit and save it so that it contains the following two lines. If you already did *Example #1*, the file may already contain this:

  700 3000
  0 NA(0.5)K(0.5)AL(1.0)SI(3.0)O(8.0)SI(10)O(20)H(20)O(10) *

2. Create another file (for this example, I call it *therend.txt* but you can name it anything you wish) that contains a single line that contains "TP" (without quotes), the final T, the final P for calculations and the number of points between, followed by a blank line. For example, *therend.txt* might contain 2 lines (second one blank):

  TP   1000   10000   6

  If you start Theriak and enter these responses, you will get results at 6 different TP conditions:
    database   *jun92.bs*   *<= you are selecting the **jun92.bs** database*
    type of calculation *therend.txt*   <= the file specifying the end of the TP path

  Calculations are done at:
    750°-3000 bars, 800°-3000 bars, 850°-3000 bars, 900°-3000 bars, 950°-3000 bars, 1000°-3000 bars

  Note: the final calculation will be at the conditions specified in *therend.txt*, but initial calculation is at 750°, not 700°, i.e., the values in *therin.txt* are NOT the first used for the calculations.

  *The output from Theriak that you saw on the screen is also in the file *thkout.txt* – making it easy to grab values and put them in a spread sheet or whatever else you want to do.

Example Calculation #3 (Theriak with long output and oxygen calculated from charge balance)

1. Go to the *Working* folder and open *therin.txt*. Edit and save it so that it contains these two lines:

    600 4000
    1 SI(60)AL(60)NA(10)K(10)SI(100)H(100)O(?) *   <= *note the 1 and the question mark*

    (Note: elemental symbols <u>must be in all caps</u> – easy to forget, and if you forget the program will produce a "fatal error.")

    T and P are 600 °C and 4000 bar The bulk composition corresponds to 10 muscovite + 10 paragonite with excess SiO2 and water. The "?" for oxygen means that oxygen is calculated from charge balance. The "1" at the beginning of the second line produces a longer output and the star "*" at the end means, that all matching phases in the database are to be considered.

2. Run Theriak as above in Example 1.

    The results first list the input data, then the phases being considered and compositions, then the solution models that are used. After that the equilibrium assemblage is listed (number of moles of each phase) and also the compositions of the solid-solution minerals.

    In this case, the result is 60.1% quartz, 23.1% H2O, 8.9% white mica, 3.9% feldspar, and 3.9% sillimanite. The mica is 70.1% muscovite, and the feldspar is 96.2% albite.

    *The output from Theriak that you saw on the screen is also in the file *thkout.txt* – making it easy to grab values and put them in a spread sheet or whatever else you want to do.

Example Calculation #4 (Domino)

1. Go to the *Working* folder and open *therin.txt*. Edit and save it so that it contains the same composition as in Example #2. (If you did *Example Calculation #2*, then the composition is already correct.) But, change the "1" on the second line to a "0", so the output will be short. It should look like this:

        600 4000
        0 SI(60)AL(60)NA(10)K(10)SI(100)H(100)O(?) *

> The T and P values have no meaning for this calculation but are included as space fillers so that all input for Theriak and Domino have the same format.

Double click on start.bat and start Domino by typing "domino" followed by a CR; then enter the following responses (**that are in bold below**) at the prompts. (Alternatively, hit CR for the default responses if the correct ones are already there.):

[database]	*jun92.bs*	<= *you are selecting the **jun92.bs** database*
[X-axis]	**tc 500 900**	<= *T range for phase diagram*
[Y-axis]	**p 1000 13000**	<= *P range for phase diagram*
[Calculation type]	**.**	<= *a period means normal calculations*
[labeling of reactions]	**1**	<= *standard reaction labels*

> ****Note that there must be <u>two</u> spaces between TC and 500, 500 and 900, P and 1000, 1000 and 1300. (I am not sure why, but a single space between values does not work!)**

> Domino should now start doing calculations – some intermediate output will scroll by on your screen until it is done. These calculations take 10 seconds on my computer.

> When Domino is done, you will be back at the command prompt. Output is in three files: *domout.txt*, *coplot*, *domino.last*. But the output is not very meaningful – a phase diagram is needed.

2. To clean up labels and then plot a phase diagram, you must run Guzzler and Explot.

> In the console window, type "guzzler" followed by a CR, then enter the following (**in bold below**) responses at the prompts:

[graphics input file]	*coplot*	<= *data comes from Domino output*
[size of labels	**0.2**	<= *label size is 0.2"*
[options]	**<CR>**	<= *just hit CR because you need no options*

> Guzzler runs quickly. Output is in a file called *clean*. Other output files are *gitter*, *table*, and *guzzler.last*.

3. Now make a plot: in the console window, type "explot" followed by a CR, then enter the following (**in bold**) response at the prompt:

        [graphics input file]   **clean**   <= data comes from Guzzler output

> Explot runs quickly and output goes into a postscript file called *plot.ps*. Other output goes into a file called *explot.last*.

4. To see the phase diagram, you must open *plot.ps*. This is a postscript file and will open in whatever program you have set up as the default for such files. (Typically that will be *Photoshop*, or *Adobe Illustrator*, but others are possible.)

> Go to the *Working* folder and double click on *plot.ps* to open it.
> You will see a complicated equilibrium phase diagram with some reactions numbered instead of labeled (because there is not enough room for labels.) To see a list of reactions and numbers, open the file *table* in the *Working* folder.