

EARTH 438 - Advanced Topics in Geophysics (C.R. Bina, 2017)

Basic Exercises in the Use of the Perple_X Code
(cf. [Connolly, 1990, 2005, 2009](#); [Connolly and Kerrick, 1987](#); [Connolly and Petrini, 2002](#); etc.)

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exercise 8 updated 2021-06-01-crb

Installation

Install the [Perple_X](#) software (current version 6.7.9 or 6.8.0) on your computer. Note that this is old-school software, largely command-line driven without graphical user interfaces.

- Linux executables available as gzipped tar file [here](#);
- Mac executables available as zip file [here](#);
- Windows executables available as zip file [here](#);
- Data files available as zip file [here](#);
- Fortran sources (not necessary - only for the curious) available [here](#).

Perple_X Example 1 (Earth 438, C.R. Bina, 2017)

After installing Perple_X:

1) Use "build" to construct an input file for the following simple problem.

- thermodynamic data file: stx11ver.dat
- computational option file: accept default
- transform components: no
- saturated components: no
- chemical potentials as independent variables: no
- **select components: MGO, SIO2**
- computational mode: accept default
- dependent potentials: no
- x-axis: P (range: 1 to 3e+05 bar)
- T range: 300 to 2300 K
- specify by weight: no
- **molar composition: 100% Mg2SiO4**
- print file: yes
- exclude pure phases: no
- include solution models: no

2) Use "vertex" to find equilibrium by free-energy minimization.

3) Use "pssect" to plot the resulting P-T section. View and print the PostScript file.

How do your results compare to Figure 6 of [Stixrude and Lithgow-Bertelloni \(2011\)](#)? How do they compare to the ancient Figure 1a of [Bina and Liu \(1995\)](#)?

4) Use "werami" to find the following properties at conditions of (230 kbar, 2000 K) and at conditions of (240 kbar, 2000 K).

- phases present and their relative proportions by volume
- compositions of each of the phases present
- density of the assemblage
- Poisson's ratio for the assemblage

Perple_X Example 2 (Earth 438, C.R. Bina, 2017)

1) Use "build" to construct an input file for the following slightly less simple problem.

- select components: MGO, SIO2, FEO
- molar composition: 90% Mg₂SiO₄ + 10% Fe₂SiO₄
- include solution models: yes
- solution model file: stx11_solution_model.dat
- select solution models: O, Wad, Ring, Wus, Aki, Pv

2) Use "vertex" to find equilibrium by free-energy minimization.

3) Use "pssect" to plot the resulting P-T section. View and print the PostScript file.

How do your results compare to the ancient Figure 1b of [Bina and Liu \(1995\)](#) or to the even older Figure 1 of [Ita and Stixrude \(1992\)](#)?

4) Use "werami" to find the following properties at conditions of (230 kbar, 2000 K) and (240 kbar, 2000 K).

- phases present and their relative proportions by volume
- compositions of each of the phases present
- density of the assemblage
- Poisson's ratio for the assemblage

5) Answer the following question, based on your results. When the phases ferromagnesian silicate perovskite (bridgmanite) and magnesiowüstite (ferropericlase) coexist in equilibrium, into which phase does iron partition more strongly?

Perple_X Example 3 (Earth 438, C.R. Bina, 2017)

Starting from your successful results in Example 2, modify it to approximate a case in which olivine persists metastably, so that wadsleyite never forms. To do this, you will need to add both "wad" and "fwad" to the "excluded phase list". You can accomplish this simply by running "build" again, or (if you are feeling brave) you can just use a text editor to edit a copy of "example2.dat" to produce a suitable "example3.dat" file.

Answer the following questions, based on your results, by comparing the phase diagram for example 3 with that from example 2.

1. What happens to the ringwoodite field at low temperatures?
2. What happens to the ringwoodite field at high temperatures?
3. What happens to the olivine field at low temperatures?
4. What happens to the olivine field at high temperatures?
5. Examine question 4 in detail by using "werami" to compare the phase assemblages at (145 kbar, 1900 K) for example 3 vs. example 2.

How do your results compare to Figure 9 of [Walton et al. \(2014\)](#)?

Perple_X Example 4 (Earth 438, C.R. Bina, 2017)

You will now pursue a model similar to Example 2, except that you will seek to create a P-X diagram instead of a P-T diagram. For the bulk compositions, instead of an Fo₉₀ olivine composition, however, you will return to the eclogite-garnetite transition whereby enstatite dissolves into pyrope to form a garnet-majorite solid solution. You should run "build" again, to create a suitable "example4.dat" file.

Your instructions to "build" will be similar to those in Example 2, except for the following major changes.

- The chemical components needed are MGO, SIO₂, and AL₂O₃.
- The x-axis variable will be option 3: "Composition X(C1)* (user defined)".
- The y-axis variable will be P, with a range of 1 bar to 220 kbar.
- Temperature will be fixed at 1300 K.
- Compositions along the x-axis will range from C0=Mg₄Si₄O₁₂ to C1=Mg₃Al₂Si₃O₁₂.
- You need to include the following solution models: Opx, Aki, Gt.

Plot the resulting P-X phase diagram.

How do your results compare to Figure 6 of [Zhang and Liou \(2003\)](#)? How do they compare to the ancient Figure 1a of [Bina and Wood \(1984\)](#) or to its precursor Figure 3 of [Akaogi and Akimoto \(1977\)](#) recently reprinted as Figure 4 of [Akaogi \(2016\)](#)?

After you are convinced that you have constructed the correct phase diagram, if you are feeling ambitious, you can try to improve the resolution of your phase boundaries by changing some of the [Perple_X options](#) from their default values in the "perplex_option.dat" file. Some values that I have found useful for such purposes include:

- auto_refine_factor_I → 6
- auto_refine_factor_II → 8
- final_resolution → 1.0e-4 1.0e-4
- initial_resolution → 1/30
- solvus_tolerance_II → 0.1

PerpleX Example 5 (Earth 438, C.R. Bina, 2017)

You will now pursue another model similar to Example 2, except that you will use a more complex composition. The "pyrolite" model is a family of compositions initially proposed by [Ringwood \(1962\)](#) as a likely composition for Earth's upper mantle, consisting of roughly one part basalt to four parts dunite. (The name is derived from **pyroxene** and **olivine**.) There are many different estimates of "pyrolite" compositions. You will use one devised by [Stixrude and Lithgow-Bertelloni \(2005\)](#) ("Pyrolite" from their Table 1) as a highly simplified version of a composition proposed by [Ringwood \(1979\)](#).

Your instructions to "build" will be similar to those in Example 2, except for the following changes.

- The chemical components needed are SiO₂, MgO, FeO, CaO, and Al₂O₃. (For brevity, NaO was neglected while simplifying this particular "pyrolite" model.)
- The x-axis variable will be P, with a range of 1 bar to 300 kbar.
- The y-axis variable will be T, with a range of 300 K to 2800 K.
- You will include all of the solution models offered, with one exception. For garnet-majorite, you will choose the full Gt_maj solution, ignoring both the simpler Gt and Gt_cmaj solutions.

Use "pssect" to plot the resulting P-T phase diagram.

How do your results compare to Figure 16 of [Stixrude and Lithgow-Bertelloni \(2011\)](#)?

Answer the following questions:

1) At high temperatures ($T > 1880$ K), at approximately what pressure is the transition to a simple three-phase assemblage of ferromagnesian silicate perovskite + magnesiowüstite + calcium silicate perovskite complete?

2) At lower temperatures ($800 \text{ K} < T < 1880 \text{ K}$), what is the stable phase assemblage at these same pressures?

3) Use "werami" to generate a 2-D grid of density values across your P-T space, using a grid density of 100x100 points. Then use "pstable" to plot a contour diagram of density from the resulting table file (probably named something like "example5_1.tab"), using a contour interval of 100 kg/m³. Which reaction gives rise to the most rapid change in density in the entire P-T space? (The simplest way to do this may involve overlaying your density-contour plot on top of your phase-diagram plot and stabbing your pencil through the paper at the point(s) of maximum density gradient...)

PerpleX Example 6 (Earth 438, C.R. Bina, 2017)

You will now pursue a P-X diagram similar to Example 4, except for two major changes. Firstly, for the bulk compositions, instead of a range of pyroxene-garnet compositions from $\text{Mg}_4\text{Si}_4\text{O}_{12}$ to $\text{Mg}_3\text{Al}_2\text{Si}_3\text{O}_{12}$, you will model a range of olivine compositions from Mg_2SiO_4 to Fe_2SiO_4 . Secondly, and perhaps more importantly, you will not construct the common isothermal P-X diagram in which temperature is fixed at some constant value. Instead, you will construct an adiabatic P-X diagram, in which temperature varies as a function of pressure along a geotherm that approximates a mantle adiabat.

In this case, we will adopt a simple model of an upper mantle adiabat from [Katsura et al. \(2010\)](#) which can be closely approximated by the linear function: $T[\text{K}] = 1720 + 0.4 * (z[\text{km}] - 200)$. To convert this to a function of pressure, you may assume the rough approximation: $z[\text{km}] = 3 * P[\text{kbar}]$. To enter this geotherm into Perple_X, you will have to write it in the form: $T[\text{K}] = a_0 + a_1 * P[\text{bar}]$.

You should run "build" again, to create a suitable "example6.dat" file, allowing pressure to vary along the y-axis from 70 kbar to 200 kbar.

Use "vertex" to determine the equilibrium assemblages, and use "pssect" to plot the resulting P-X phase diagram.

- What happens to very iron-rich ringwoodite at around 560 km depth along such a geotherm?

Use "werami" to produce a 1-D table of phase modes for a Fo_{90} composition, along this adiabat.

- For such a composition, along such a geotherm, at what depth does wadsleyite first appear? At what depth does olivine finally vanish?

PerpleX Example 7 (Earth 438, C.R. Bina, 2017)

You will now return to the pyrolite model of Example 5, but you will combine it with the geotherm of Example 6 and more sophisticated use of “werami” and “pstable”.

Run “build” again to create an “example7.dat” input file. This time you will ask for minimization on a 1-D grid (essentially a single P-T path) rather than the usual 2-D grid. You will specify the pyrolite bulk composition from Example 5 and Katsura’s adiabatic geotherm from Example 6. As in Example 7, you will enable all of the solution models (while selecting only Gt_maj, instead of Gt or Gt_cmaj, for garnet). Choose a pressure range from 50 kbar to 220 kbar.

Run “vertex” to obtain the equilibrium assemblages, and then run “pssect” to plot those assemblages.

Now run “werami” to extract properties along a 1-D path, with pressure ranging from 50 kbar to 220 kbar and a grid spacing of 1 kbar. You want to extract the compositions of solution phases. First specify olivine (O) composition ($fo/[fo+fa]$), then specify wadsleyite composition ($wad/[wad+fwad]$), and finally specify ringwoodite composition ($ring/[ring+fring]$). This should generate a “example7_1.tab” file containing the compositions of these three phases in three separate columns.

Finally, run “pstable” to plot the compositions of all three of these phases as functions of pressure. To see more detail, you probably want to modify the default plot so that the y-axis values range from 0.85 to 1.00 (instead of using the default range that starts from zero).

What happens to the composition of olivine with increasing depth in this pyrolite composition? What happens to the compositions of olivine and its polymorphs near their divariant phase transitions? How does this compare with the observations of [Irifune and Isshiki \(1998\)](#) and the accompanying commentary by [Bina \(1998\)](#)?

If you are feeling particularly ambitious, run “werami” again to extract the fraction of majorite in the garnet-majorite solid solution for this pyrolite composition along this P-T path (thereby creating a “example7_2.tab” file), and use “pstable” to plot it. What happens to the fraction of majorite in garnet at pressures above ~190 kbar? Why? (You may have to go back and study your plot from “pssect” above to figure this out...)

PerpleX Example 8 (Earth 438, C.R. Bina, 2017, 2021)

You will now pursue another exercise similar to Example 7, but instead of a 1-D gridded minimization specifying $T(P)$ in polynomial form, you will first perform a 2-D gridded minimization and then specify a series of specific (P,T) points which trace a self-consistent adiabat.

First, run “vertex” to perform a 2-D gridded minimization on a pyrolite composition over a P range of 1 bar to 300 kbar and a T range of 300 K to 2800 K (essentially identical to Example 5). You may wish to run “pssect”, too, to confirm that your resulting P-T diagram looks like the one that you made for Example 5.

Then, run “werami” to extract the entropy S (J/K/kg) for the total assemblage on a 2-D grid into the file “example8_1.tab”. You will probably want to select a grid density of something like 157x157 nodes. If you choose a denser grid (something like 313x313 nodes), you probably will exceed the default array dimensions, and strange errors will occur as you overwrite memory. (To make this work with such a denser grid, you first would have to increase the parameters “nx” and “ny” in the Perple_X source file “perplex_parameters.h” and then recompile the source code. For such purposes, I sometimes increase them to 1500, from their default values of 500.)

Now we need to choose an entropy value to define our adiabat. The Katsura geotherm that you used earlier specifies a temperature of 1800 K at a pressure of 133333 bar, and a temperature of 1900 K at a pressure of 216667 bar. For simplicity, we will try to choose an adiabat that closely approaches these two points. Use “werami” to determine the value of entropy S at each of these two points, and then find the mean of these two entropy values. This fixed entropy value will define our adiabat.

Next, use “pstable” to plot a contour of S at this single fixed value. In order to plot this single contour line, you will need to modify the default plot slightly. Modify the default contour interval so that the minimum and maximum values are both set identically to your chosen value of S , with a contour interval of 1. Echo the resulting contour data to file “contor.dat”.

Now take a look at your resulting “example8_1.ps” graph. This shows a curve of constant S in P-T space, at your chosen value of S . (Note that the curve sometimes may appear a little jagged across very sharp transitions, especially if the width of the transition is similar to or less than your grid spacing in P-T space; perhaps you could fix this by using a denser grid.) Such a curve of constant S is a true, self-consistent adiabat (because, under conditions of thermodynamic equilibrium, $\delta q = TdS$, and for an adiabatic system, the heat flow $\delta q = 0$; thus, $dS = 0$). Notice how, unlike the simple approximation you used before, this is not a simple polynomial curve. Notice how it "refracts" across regions of phase transition (due to the non-zero ΔS of reaction).

What is the direction (increasing or decreasing T) of refraction across the olivine → wadsleyite transition? How about the wadsleyite → ringwoodite transition? What about the bridgmanite-forming

transition(s)? You may wish to compare your curve with the solid line in Figure 2 of [Bina \(1998\)](#) and to reflect upon the several reasons for any apparent differences.

Next, make a copy of the “contor.dat” file, named as “contor_edit.dat”. In principle, your file should contain the coordinates of a single contour in a single long segment. However, sometimes one or more additional small segments (each beginning with the word "segment") are appended, apparently due to rounding errors in the contouring algorithm. Use your favorite text editor to modify “contor_edit.dat”, deleting anything after the end of the first long segment. Also, delete the two text-bearing lines at the top, so that the file contains only (T,P) points.

Now we must swap the (T,P) columns to give (P,T) points (e.g., "awk '{ print \$2, \$1}' contor_edit.dat > contor_swap.dat"). Your resulting “contor_swap.dat” file may have its lines organized by increasing pressure or by decreasing pressure. You can sort the lines of the file numerically to make sure they are organized by increasing pressure (e.g., "sort -n contor_swap.dat > contor_sort.dat").” Now you should have a “contor_sort.dat” file containing only unique (P,T) points sorted by increasing pressure.

Sometimes adiabats are casually described in terms of their “foot” temperature, which is the temperature that they achieve at some reference pressure, typically of 1 bar. Note that the foot temperature of the Katsura geotherm is 1640 K. What is the foot temperature of your adiabat?

Finally, you can use this adiabatic P-T path to extract properties along the path. For example, you can plot the modes (in volume percent) of the phases olivine, wadsleyite, ringwoodite, and garnet-majorite along this adiabat, but this time you will use “werami” to extract properties along a 1-D path that is specified from your input file named “contor_sort.dat” containing x-y (P,T) points. The resulting file (e.g., “example8_2.tab”) can be plotted using “pstable”, just as in Example 7. You may want to modify the default plot, to make sure that the y-axis (volume percent) range is set to 0-100.

Alternatively, you can plot the compositions of the solution phases olivine, wadsleyite, and ringwoodite along this adiabat, just as you did along the Katsura geotherm in Example 7.