

Phase Diagram Computation (Perple_X) and Elementary Thermodynamic Principles

The course is currently scheduled as four three-hour meetings, which are to be split between lecture and practical. Phase diagram computation is fundamentally an optimization problem. My intention is to use the first meeting to introduce the basic optimization problem and Perple_X, one, among many, of its practical solutions. This introduction should motivate more fundamental questions to be answered in the second part of the course, such as: how the Gibbs energy, G , is derived from the first and second laws; how G is manipulated to obtain functions such as seismic wave speed and the adiabatic geothermal gradient; and how, practically, G is evaluated for pure and impure phases. These questions will serve as the basis for problems to be solved in the remaining practicals. The second part of the course assumes basic mathematical skills, notably, differentiation and integration, and some prior exposure to thermodynamic concepts.

The script for the first practical of the HUJI course is at perplex.ethz.ch/perplex/tutorial/huji_tutorial. To reiterate what is written at the beginning of that script: I recommend you copy Perple_X and verify that it runs on your computer before the course begins.

The second part of the HUJI course will be a distillation and simplification of a course that I gave at the ETH. The script of that course is at perplex.ethz.ch/thermo_course. Problems 1.1-1.4, 4.5-4.8, 5.1-5.2, and 8.1 in that script (thermos_course.pdf) are representative of, if not identical to, the material that I plan to cover at HUJI. There are helper scripts for some of the problems written for a symbolic math tool named Maple. Use of alternative symbolic math packages, such as Python, Mathematica, or Matlab for the HUJI course is fine; however, if you are interested in using Maple, the first page of the ETH course script describes how you can obtain it.

Nothing about this course is written in stone, the number of meetings can be reduced or increased, the content adjusted, and the ratio of lecture to practical time varied according to the wishes of the participants. Throughout my career I have consistently overestimated what I am capable of teaching effectively, so please do not be shy about making suggestions.