Applied Statistical and Numerical Methods
for Materials Scientists and Engineers

an undergraduate course
offered at the University of Tennessee, Knoxville
MSE 301
Fall, 2017

taught by
Prof. David J. Keffer

This course is equally divided into two topics: Applied Statistical Methods and Applied Numerical Methods. In both cases, the approach is to present the basic mathematical theory and then provide practical, hands-on application of the theory relevant to Materials Scientists and Engineers. The course empowers the undergraduate student by allowing them to see for themselves that many statistical and numerical tasks that at first seem daunting in their mathematical complexity are in fact quite straight-forward to accomplish using standard commercial software that is available today. The course requires a working familiarity with MatLab. However, extensive programming is not required. Rather, one uses and modifies existing codes to meet the needs of a particular problem. The course will include a materials-oriented project, such as the creation of a eutectic phase diagram from the evaluation of regular solution theory.

When the student emerges from this course, they will know that the most difficult part of a materials problem is no longer in the numerical evaluation of the model but rather in the much more interesting formulation of the model, such that it captures the phenomena of interest. They will be confidently able to state, "If I can write the equations that describe the material, I can solve the problem."

From 1998 to 2003, Prof. Keffer taught MSE/ChE 301, which was required by the MSE department at the time and covered much of this material. The offering of a modified version of the course was resumed in 2014. Students interested in further information are encouraged visit the course website, which contains a syllabus and lecture notes. That website is located at http://utkstair.org/clausius/docs/mse301/index.html.

$$\Delta G_{mix}^{j}(T, x_A) = \Omega^j x_A (1 - x_A) + kT \sum_i x_i \ln(x_i)$$

An example of the capabilities developed in this class: Generating a eutectic phase diagram from regular solution theory. One has two equations describing (i) the free energy of mixing from regular solution theory and (ii) the thermodynamic constraints of phase equilibrium. Taken together, they provide all necessary information to generate the phase diagram. The actual numerical construction of the phase diagram is straight-forward once a student has the appropriate tools in hand.