

Syllabus
Computational Chemistry
Chemistry 443/543
Fall 2010

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Office Hours: Monday, Tuesday, Wednesday 9:30 – 10:30 a.m.

Background The objective of this class is to familiarize the student with a powerful concept in modern computing: the prevalence of high-level computational tools (*e.g.*, MatLab, Maple, Excel) and pre-built routines (often available from the WWW) to execute within them makes it possible for chemists to do MOST of the mathematical/computing work that we need to do with at most minimal modifications to existing routines. Some of the programs are even graphical in nature making the programming very intuitive. Most programs that we will use also incorporate visualization tools that allow you to make more or less complicated graphical representations of the data.

Grading The entire grade for the course will be based on projects (exercises) that you will complete on your own (on your own computer, if you wish, wherever you choose to work, and at whatever pace you wish to keep.) For the graduate student version of the course, one of the projects will require you to go beyond the parameters that are required, and in this case you will need to meet with the instructor at an arranged scheduled time to present the motivation, mathematical strategy, and the algorithm that you developed for addressing the “extended exercise” project. You will also need to get authorization for this project from the instructor, optimally before you start work on it.

Lecture The lecture only exists to support the work you will do (by yourselves and when and wherever you like, for the most part) on the exercises. There will not be any tests or quizzes in this class; your grade is entirely based on the successful completion of the exercises that are described in greater detail below. The support provided during the lecture will include the concepts behind the exercises and some help actually getting started (we have computers in the hybrid classroom but you can also bring your laptop and work there.)

Exercises The programming exercises are available on the web via the Desire2Learn (a.k.a. D2L) site. You will also turn in your work via the “Dropbox” tool online and will receive grades and feedback from the instructor via the same tool. It is advisable to turn in the exercises in a timely fashion, since the instructor will provide you with the feedback in an equally timely fashion (generally within one week) and you can avoid making the same mistake more than once by using the feedback to improve your performance.

The exercises are downloaded from the D2L site and opened in MS Word. If you are inserting figures from another software package and they appear to be problematic, try changing them (Save As, or Export) to pictures (WMF, JPEG, etc.) or pdf formats and then insert them in the Word document. If you like Excel, the graphs that are made in Excel nearly always copy into Word with little or no difficulty.

The exercises are color coded to help you identify the important parts of the document. Black text like this is just general background material to help you understand the motivation for the problems that we are doing and the approaches that you might take to solve the problems. In each case, we will suggest a route to the solution of the problem, including some “tune-up” exercises that you can do for credit and also to familiarize yourself with the program that I am suggesting. You can choose to do any of the exercises in any program that you want, but if you choose to use a different program and/or approach, you are on your own in developing the solution. **Bold** and *italic* text will be used in some exercises to emphasize material, or to identify operations, for example to identify menu options in a program. **Blue text is annotations or asides, material that is interesting, but not really necessary to address the problem at hand.**

Red text is used to identify questions within the exercise that you have to answer. It is helpful if you either use the Word “Track Changes” tool or use a different font color for your answers. Note that you have to answer all of the questions in the exercise, regardless of the approach/program that you choose to use to address the problem in the exercise. This means that you may have to do some of the intermediate “tune-up” exercises to obtain the answers. Sometimes the answer will be a few words or a sentence or two, and sometimes the answer will be a graph or a table. It should be obvious what is required from the context.

Green text is used to identify the programming exercises that you will need to do. In every case, this will require you to switch to or launch another program to complete the actual programming and extraction of data. It should be possible to have both programs open at the same time and switch back and forth (or set up a split screen) so that you can follow directions (when applicable). There will almost always be red **questions** associated with the green **programming exercises**.

Don’t forget to save your file with your initials (e.g., SpectralFit_DBA.xls) and to save it fairly often, in case you make irretrievable errors or the computer crashes. “The computer ate my homework” will not be considered an acceptable excuse in any case.

Copying others work In order to make the course meaningful, we have to ask that you work on your own problems. Obviously, you can discuss the general parameters of the solutions with others in the class and strategies that you and others used to address them; but when you actually sit down to do the exercises, it needs to be you working alone. If the instructor suspects that you either started with someone else’s work or got someone else to do your work for you, they may call you in for a consultation at any point during the term at their discretion. Generally speaking, a person will remember what they did during a programming project and if you don’t, it will be taken as evidence that you didn’t do the work. At the discretion of the instructor, you may lose credit for one or more exercises in that case.