Syllabus
Chemistry 443/543 Computational Chemistry
Fall 2011 – SRTC B1 82 (MW 4:30 – 6:30 p.m.)

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

Background  The objective of this class is to familiarize students with a powerful concept in modern computing that I’ll call “easy math”. The prevalence of high-level computational tools (e.g., Excel, MatLab, or LabView) and pre-built routines (often available on the web) 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 part very intuitive. The programs that we will use also incorporate visualization tools that allow you to make more or less complicated graphical representations of the data with little effort.

Grading  The entire grade for the course will be based on projects (called Exercises) that you will complete on your own (on your own computer, if you wish). For the graduate student version of the course, one of the projects will require you to design your own Exercise, and in this case you will need to meet with the instructor to discuss the motivation, mathematical strategy, and the algorithm that you plan to use for addressing this “extended exercise” project.

Lecture  The lecture only exists to support the work you will do (by yourselves and whenever 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 required exercises (described in greater detail below). The support provided during my lectures will include the concepts behind the exercises and some help actually getting started with the programming. There are recorded versions of the lectures available on the Desire2Learn (a.k.a. D2L) site, via the Elluminate tool.

Exercises  The programming exercises (in MS Word format) are available on the web via the D2L site in the Course Content section. You will also turn in your work online via D2L’s Dropbox tool 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 can then 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.

Deadlines  In a perfect world, we wouldn’t need deadlines. But a couple of years of experience with this class provided ample evidence that we do need them in this case. Starting with the Friday of the second week of classes, there will be one exercise due each week. If the exercise is submitted to the Dropbox after Friday at midnight (the time and date are recorded...
when you submit) it will begin to accrue late points (one point is lost per weekday that it is late, out of a total of ten points per Exercise, so a Monday submission would be worth 9 points total, while a submission on the following Friday – one week late – would only be worth a maximum of 5 points). You can turn in (and work on) the Exercises in any order you want, so the first one you turn in might be Exercise 4 and the one the following week Exercise 1, but you HAVE to turn in one each week after the first (grace) week. When I wrote the exercises, I put more explanation in the first few about how things work, but they are also some of the harder ones.

**Where can I work?** The lecture will be given at the beginning of class time on Mondays in SRTC (used to be Science Building 2) B1 82 and then you can work in this room until 6:30 p.m. We will also have this classroom open and staffed by a TA on Wednesday from 4:30 to 6:30 p.m. You don’t have to work in this room or on the desktop computers there, but they do have most of the programs installed and the TA can be quite helpful. If you choose to work on your own computer, we can’t guarantee that all of the recommended software will be available for you to use. For the Spartan project (Exercise 8) only the computers in the ChemCommons have licenses for this software. If you treat this course like any other lab class and come every MW, you will easily finish the Exercises with time to spare.

**Getting going** The exercises are downloaded from the D2L site and opened in MS Word. If you are inserting figures from another software package and they don’t look right, try changing them (Save As, or Export) to pictures (WMF, JPEG, etc.) or pdf formats and then insert them in the Word document. 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 general, I will suggest a route to the solution of the problem, including some “tune-up” exercises that you can do for credit and to familiarize yourself with the program that I suggest you use. In each case, there will be a final product (or products) for the exercise. 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 denotes 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. 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. It is helpful if you 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.

**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.