Chem 8843: Mathematical Methods for Chemistry

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Office Hours: by appointment

Course Material: Common mathematical methods used in data simulation, modeling, and analysis. You will be responsible for all class and supplemental material provided during the semester. Class attendance is strongly recommended. Class will heavily utilize Mathematica software.

Class time: Tuesday-Thursday 9:35 - 10:55AM, MS&E G021

Textbook: Mary L. Boas, *Mathematical Methods in the Physical Sciences*, 3rd Edition, John Wiley & Sons, Inc., 2006

Prerequisites: Knowledge of Calculus, Linear Algebra, Differential Equations

Grading: Homeworks/class participation (30%), two group projects modeling research papers to be completed in Mathematica (20% each) and a 3rd individual project (30%) will comprise the grade. The third project is in lieu of a final exam. Mathematica will be used throughout the course. If you can bring a laptop to class, that is ideal, as we will work through problems in class. All students are responsible for material presented in class and in the required textbooks. You will be expected to present specific topics in class as well.

Homework: Homework will be assigned occasionally, with a specified due date. Homework must be submitted electronically through t-square. It is expected that everyone will do the homework, this is the only way to learn the material. Working with others is encouraged in the understanding of the homework problems and class material; please, however, make sure that you understand the problems and that the problems you turn in are your own work.

Honor Code.   Projects should be your own work, and all sources (literature, people, reference material) should be cited.

Software: Georgia Tech has a site license for Mathematica, and a student version can be downloaded for free from the software page at www.oit.gatech.edu. Do this immediately as it will take up to a few days to get a license for your machine. Many resources are available at www.wolfram.com. The extensive help files within Mathematica are also very useful.

Scope: It is expected that this course will help accelerate the pace of and improve success within your other graduate courses. It is also expected that upon starting in a research group, everyone will be able to quickly model ongoing experiments, improving our overall research effort and success.