Alleviating computational anxiety of chemistry students

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I recently started a tenure-track position at Fresno State in the chemistry department. Currently, I am teaching a computational chemistry course at the master's level. One thing that I noticed immediately was the anxiety many of my students expressed about the math that would be involved. Although I certainly expected this reaction to some degree, I was still surprised by the trepidation and dread of the required mathematics and computational knowledge they expressed on the first day of class. Additionally, during what was supposed to be a brief review of linear algebra, I was taken aback by the fact that about half were unfamiliar with basic matrix multiplication, and the representation of linear equations. These students are generally quite comfortable with basic integration and differentiation, but unfamiliar with numerical methods and translating abstract theory into useful results. This has highlighted the need for more emphasis on computational skills, and particularly the need for an emphasis on practical application of these skills within chemistry.

By its nature, chemistry involves quite a bit of quantitative reasoning. In introductory courses, students encounter concepts like stoichiometry, the gas laws and equilibria, all of which require some degree of computation. This material becomes more complex in upper division classes such as analytical or physical chemistry, and many times these courses are simply seen as something to "survive". Generally, it is the mathematics and computational aspects of these courses that cause stress for students, rather than the chemical concepts. In my graduate course when I told them they would not have to find the eigenvalues of a matrix by hand there was a collective sigh of relief. However, knowing how to solve for these values using MATLAB or iPython or Mathematica was also beyond their experience. By introducing them to tools used for solving equations, I believe it has already reduced some of the anxiety surrounding the course.

Even in subdisciplines such as organic chemistry, which are traditionally seen as not requiring significant computation, the underlying skills are similar. I am also teaching an undergraduate organic chemistry this semester, and there I have found that my students there struggle with complex problem solving. The skills needed to parse information and propose reaction sequences are very similar to those needed for computational work. I have often found that there is a significant disconnect for students between knowing the reactions and being able to apply them appropriately, and the anxiety surrounding synthesis problems is similar to that surrounding computational problems. There are also opportunities to introduce computation into such courses. As I am fairly new to teaching, this year I brought in a computed model system for visualizing vibrational frequencies in molecules which they found quite interesting, and it helped clarify the concept for them. Next time I teach the class though I would like to have them run such model calculations themselves. There is something very powerful in being able to visualize molecules through the computer, and it excites students when they realize what they can do with computational modeling.

Computational skills are used throughout the chemistry curriculum, but frequently underemphasized. Their utility is recognized to a minimal degree by the American Chemical Society (ACS). However, while ACS guidelines for undergraduate degree programs discuss the need for the availability of computational facilities and software, and that they should be incorporated into the laboratory curriculum, they give no explicit guidance on the extent to which this should be done (in contrast to other subdisciplines such as organic or analytical chemistry).

The ability to compute chemical properties and phenomena complements experimental work by enhancing understanding and providing predictive power. Students should have access to computing facilities and use computational chemistry software.

The laboratory experience must include, measurement of chemical properties, determination of structures, hands-on experience with modern instrumentation such as that listed in Section 4.2, data analysis, and computational modeling. [1]

Thus, student exposure to computational approaches is usually minimal at best, and does not include any need to understand the underlying principles of the codes or how to apply and modify them appropriately. Again, the need to understand the theory and operation of instruments such as IR (infrared) and NMR (nuclear magnetic resonance) spectrometers, and other standard tools is explicitly specified, this does not extend to computational work.

Laboratory experiences should be designed to teach students to understand the operation and theory of modern instruments and use them to solve chemical problems. [1]

The “modern instruments”, are specifically listed in a different section of the document than the statements about the availability of computational resources. Thus, while individual departments may potentially extrapolate, for the most part students can graduate knowing very little about actual scientific computation.

I first noticed the effects of chemistry program deficiencies in computation as a graduate student. I did have significantly more experience with computation than most my peers having completed a math major in addition to my chemistry major, and taken at least an intro to computer science course. A common difficulty for those working in experimental labs was that they were expected to run scrips or write basic programs to control lasers and other instruments, or to do data analysis and often they had never experienced working with anything similar. Eventually they would figure out enough so that they could do their experiments, but much stress might have been avoided if computation and basic programing had been integrated into their undergraduate programs.

Not all students are going to be interested in pursuing theoretical and/or computational chemistry as I have done, but much can be done to alleviate some of the anxiety that accompanies using computers and numerical analysis in courses or in research for many of them. Integrating more computation into standard undergraduate courses is one way to accomplish this, but as many faculty members are also uncomfortable with the necessary computational skills this will be an ongoing challenge. I hope to do as much as possible to change this in all my courses, and as I settle into teaching prepare my students to use computational skills as much as possible for their future careers. As experimental data sets continue to grow, and instruments become ever more automated, students who are afraid of applying computational methods are at a disadvantage. One of the common strategies for dealing with anxiety disorders is exposure therapy, and by exposing students to computational tools I hope to eventually minimize their discomfort.

[1] American Chemical Society Committee on Professional Training, “Undergraduate Professional Education in Chemistry: ACS Guidelines and Evaluation Procedures for Bachelor’s Degree Programs”, ACS, Spring 2015, 38pp.