I was drawn to physical chemistry as an undergraduate but I didn’t learn much, because as a quantitative science it was, then, too difficult to work meaningful problems. We didn’t have any computational facilities at my university to facilitate working problems in those days (circa 1962). Consequently we used slide rules and math tables to work problems of the “plug and chug” variety which didn’t really reveal the most important principles.

I continued my study of physical chemistry at the graduate level and came to St. John’s in 1968 to teach it. In the 60s the Computer Center at SJU was located in Wimmer Hall. Fr. Fintan Bromenshenkel ran the Computer Center which consisted of an IBM 1620 and peripherals. The computer was used mainly for business office purposes; I was, as far as I know, the only scientific user. Jane Moening and Jeana Koenig of the Business Office were very generous in allowing me “time” on the 1620, and so I regularly trundled over to the computer center with my deck of computer cards to run some “jobs” related to a research project I was pursuing.

The IBM 1620 did not have the computational power of a currently available programmable calculator. However, even in those days I walked my students over to Wimmer Hall occasionally to demonstrate how a computer could be programmed to do a linear regression or some other simple mathematical task. I am fairly certain that these early efforts to introduce students to computers and computer applications in chemistry were not very effective. By today’s standards it was a very primitive situation.

Things improved in the middle to late 70s with the advent of interactive computers (SJU purchased a Hewlett Packard) and I began to introduce computer labs into both semesters of physical chemistry. With the hiring of a second physical chemist at about the same time, I began to concentrate my efforts on Quantum Chemistry (P.Chem. II in those days). My position on quantum mechanics then and now is that it is not as difficult as it seems if you just do it! Like anything else you learn quantum theory by using it. So I increased my efforts to develop computational exercises that illustrated and illuminated fundamental quantum mechanical principles and could be done (with comprehension) by undergraduates. I have to say in honesty that I also did this to teach myself quantum chemistry. My reasoning was that if I could calculate it, it might mean I understood; but if I couldn’t calculate it, it was certain that I didn’t understand.

My students (Nate, Ryan, and many others) were the guinea pigs in this program and I am grateful for their feed-back and patience in my efforts to develop meaningful exercises that bridge the gap between the formalism of quantum mechanics and its computational methods. The circumstance that really made a project like this feasible, of course, was the development of the personal computer and graphical user interface. Things really began to take-off in the mid-1980s. And now, they are actually superb in the sense that I have a computer lab with 11 PCs and 10 SGI workstations, several very powerful software packages to do computational quantum chemistry with my students, and excellent hardware, software, and network support from IT Services. What
more can a quantum chemist ask?

With regard to software, Mathcad is used for routine problem solving and simple quantum mechanical calculations, while Spartan is used to calculate the electronic structure and geometry of molecules. This year I have also started to use GAMESS (General Atomic and Molecular Electronic Structure System) in my Quantum Chemistry course. I have also introduced electronic structure calculations to the lower division chemistry students by preparing two computer labs for use in the general chemistry sequence. In addition I have mentored several general chemistry research projects that illustrated the use of Spartan in molecular structure calculations. However, the major effort has been in Quantum Chemistry (CHEM 334).

In what follows I will summarize the outcome of this long term effort to use computer resources and the more recently available World Wide Web to teach quantum mechanics to undergraduates. Naturally, everything I cite below (software packages, journal articles, book chapters, and tutorials) has been “road tested” by CSB/SJU students before being shared with the wider educational community through publication or Web posting. As noted above I am grateful for their perseverance, patience, and support. I should also add that student learning (and, of course, my teaching effectiveness) is also assessed with the computer. Students in Quantum Chemistry take exams, quizzes, and do their laboratory reports using the same software packages that were used to teach the concepts and methods in lecture and lab.

I have published several software packages.


- "Exercises in Quantum Mechanics", Journal of Chemical Education, 64, 789 (1987). Software distributed by Project SERAPHIM a National Science
Foundation sponsored clearinghouse for instructional microcomputer software in chemistry.

I have also published a number of articles in peer-reviewed journals outlining my computer exercises for undergraduates.

I have co-authored two chapters which outline computational methods for bringing theoretical concepts to life for undergraduates.


A complete list of publications is available at: [http://www.users.csbsju.edu/~frioux/pubs.html](http://www.users.csbsju.edu/~frioux/pubs.html).

In addition I have given the following relevant presentations at colleges and universities, and local, regional, and national meetings of scientific societies.

- "Teaching Quantum Chemistry to Undergraduates," University of Iowa, Iowa City, IA, September 9, 2002.


- "Computational Chemistry in the Undergraduate Curriculum," Red River Valley Section of the American Chemical Society, University of North Dakota, October 15, 1993.


"Using Microcomputer Graphics to Solve Schrödinger's Equation" - St. John's University; University of Minnesota-Duluth; St. Cloud State University; Fifth National Workshop of Computers in Chemistry at Atlanta University; University of North Dakota. (1981-83)


The Web provides another teaching/learning venue that I have found particularly attractive in illuminating quantum mechanical principles. I have written over fifty tutorials which are posted on my page at: [http://www.users.csbsju.edu/~frioux/workinprogress.html](http://www.users.csbsju.edu/~frioux/workinprogress.html).

I use these regularly in my classes and I like the Web-venue because it allows me to respond immediately to suggestions from readers. Some spot errors and others ask questions that stimulate further thought which leads to an improved presentation. Unlike something that has been published in print, a Web-based publication can evolve into something better immediately. The Web also enables me to teach quantum to a wider audience, and I have evidence that people, hither and yon, have read my tutorials. While the tutorials are not interactive, interactive Mathcad files are available for download for many of the tutorials.

As evidence that people off-campus are aware of my efforts in this area, I cite the fact that I was asked to organize and co-chair a three-day symposium at the American Chemical Society’s national meeting in August 2000 on “Computational Chemistry in the Undergraduate Curriculum.” In addition the editor of the Journal of Chemical Education said of one of my software packages that, "It is an electronic textbook of quantum chemistry. This is a preview of what the textbook of the future might look like."