Characteristics of a Dedicated Course on Computing in Chemistry: Form, Content and Audience

Carl H. Snyder
Chemistry Department
University of Miami
Coral Gables, FL 33124

Abstract

Beginning in the spring term, 1998, and during each subsequent spring term through 2003, the University of Miami Chemistry Department has offered "Computing in Chemistry", a three-credit course dedicated to teaching computing through the examination of chemical applications.

This paper discusses the origin of the course, its objectives, structure, content, audience, and instructors. The course was designed for science majors who had completed at least the first semester of the two-semester organic chemistry sequence, and was taught by a group of faculty with expertise in a variety of computer-related fields. Syllabi, examinations, course projects, the Web page, and related material are presented and discussed.

Introduction -- In the spring term, 1998, the Chemistry Department of the University of Miami (UM) introduced a 3-credit course in "Computing in Chemistry" with the catalog description: "Introduction to computers; information retrieval; acquisition and manipulation of data; graphics. Emphasis on chemical applications." The prerequisite was the first term of a two- semester organic chemistry sequence, with the associated laboratory.

In addition to other considerations, the course was initiated in response to a mathematics requirement for the B.S. degree that included "either a) one semester of a computer course approved by the major; or b) a statistics course approved by the major." Thus the Department's computer course offered B.S. candidates an alternative to what we perceived to be small set of unsuitable statistics courses. There were, of course, several additional, more noble and more academically sound reasons for introducing this course.

In the broadest sense, the course was designed to teach students both computer theory and practice by focusing on chemical applications, and to present a broader view of chemistry through computer applications. The course culminates in student classroom presentations of chemical information through the use of either Powerpoint or Web pages of their own creation, via a classroom computer-projector.

The course has been offered each spring term through 2003, for a total of six consecutive spring terms. The course was not offered in the spring of 2004 because of a combination of low enrollments and my own sabbatical.

Enrollments -- The course drew the following enrollments in each spring term:

[*year - total enrollment - enrollment by major*]
1998 - 5 - 3 CHM; 2 BCH
1999 - 3 - 2 CHM; 1 SOC
2000 - 7 - 3 CHM; 1 BIL; 1 CSC; 1 CSM; 1 MSX
2001 - 10 - 6 CHM; 3 BIL; 1 EES
2002 - 8 - 5 CHM; 1 BIL; 1 BCH; 1 GSC
2003 - 6 - 4 CHM; 1 BIL; 1 MSB

BCH = Biochemistry; BIL = Biology; CHM = Chemistry; CSC = Computer Science; CSM = Computer Science Mathematics; EES = Enviromental Engineering Science; GSC = Geological Sciences; MSB = Marine Science Biology; MSX = Marine Science Chemistry; SOC = Sociology

In summary, the course has drawn a total of 23 Chemistry, 6 Biology, and 3 Biochemistry majors, and one each from assorted other majors.

Form and Content - The Evolutionary Process -- For the first three terms, the 3-credit course consisted of two weekly 50-minute classroom presentations (in a classroom equipped with enough computers to give each student access to an individual computer) and one 3-hour computer laboratory. I handled the classroom presentations with the participation of several guest speakers; two departmental colleagues taught the laboratory. In practice, the classroom presentations tended to emphasize Web searching, library applications, data manipulation, Web page creation, listservers, and similar topics. The laboratory sessions emphasized hardware considerations and the use of computers in data acquisition.

Each of the two colleagues who handled the laboraratory portion of the course has left the University in the past few years. Partly because of the departure of these two colleagues and partly to strengthen the connection between the classroom presentations and the students' own computer activities, the last three terms consisted

of three weekly 50-minute sessions in the form of lecuture/workshops. These were held in the same computer/classroom as the classroom presentations of the first three semesters.

Form and Content - The 2003 Term -- The 2003 term is best described through the Web page for the course, CHM 256 B. Clicking on the palm tree graphics provides the course resources. We'll start with "Your syllabus and course information". (I recommend keeping the CHM 256 B Web page available throughout this presentation.)

The course begins with an introduction to presentation protocols, focussing on presentations 1) through Web pages and 2) with PowerPoint. I ask students to post Web presentations in their own directories on the UM student server, UMSYS. During the first week a representative of UM's Information Technology division describes UMSYS and its uses by students.

I then introduce HTML scripting and Web page preparation. Students are required to create pages by writing the script themselves. We do not use Web page authoring programs in this course. Clearly, the first **AHA!** moment comes when the students write a very simple web page ("My name is XXXXXX", with their names in red.) save it as a html file, and view it in a browser. That's the instant when the class truly begins.

Following this, we touch lightly on Powerpoint, then move on to e-mail. The director of the UM e-mail systems speaks to the class, and I have everyone subscribe to CHEMED-L, briefly, to learn about e-mail lists. (The class then unsubscribes.)

We also cover both browser- and telnet-based e-mail reading programs. In this portion I send each student an e-mail message containing the hidden name of achemical and instruct the students in using the *view page source* function of a browser to find the hidden text.

After the midterm examination there are a few workshop sessions in the library in which the director of library research instructs the class on the use of library electronic resources for information gathering. Following this a departmental physical chemist spends a week, back in the chemistry department, on chemical calculations.

At this point I should note that I am an organic chemist with strengths in mechanisms and syntheses, but a stranger to quantum and structural calculations for organic molecules. I am more graphically oriented, as becomes evident in this paper. So I leave the discussion of computer calculations to our physical chemists.

Near the end of the course we cover the creation of molecular structures, particularly MOL files, and the use of CHIME. The final few class periods are devoted to a summing up and to the student presentations. Several of the five items, noted in the syllabus, that determine the grade are described in detail in the Web page. We'll turn to them now, taking the links in sequence (except for the very first link, which is my way of introducing myself to the students . . . and illustrating how tables can enhance a Web page even though the page itself contains no explicit tabulations).

The Web Page --

The Primary Project: This is self-explanatory and is presented to the class, by the students, as Powerpoint or Web-based computer-projections.

Secondary Project 1: A text page is formatted using html script coding.

Secondary Project 2: An exercise in the interconversion of binary, decimal, and hexadecimal coding, and of the octal system.

Secondary Project 3: An early exercise in Web page creation.

Secondary Project 4: An exercise in electronic library research.

Secondary Project 5: An advanced exercise in Web page creation and in molecular graphics.

External resources . . . : Authoring and HTML coding resources. Some of these links may by now be obsolete. I haven't followed them since the course was last given.

Search tools: Links to libraries and to Google and other search engines.

Hexadecimal equivalents: A decimal-hexadecimal resource for students.

Images: Graphics and single and muliple colored pixels. We use these in Web page creation.

HTML codes for font colors: Links to hexadecimal codes for a variety of colors.

Primary additive and subtractive colors: Resources for a discussion of colors on the monitor screen.

2003 Quizzes: As the first few quizzes are given they are posted on the Web page.

For a comparison . . . : Similarities and differences between Netscape and Internet Explorer.

Hexcodes for the red A: Self-explanatory. View the source code for the correlation between the hexadecimal code for the red and the intensity of the red.

HTML tags, attributes, and acronyms: A resource for HTML coding.

Questions from CHM 256 B, Spring 2002: All the quizzes from the previous offering.

Molecular models: A substantial collection of relatively simple molecular models as MOL files.

All the spring 2003 quizzes: The entire collection of the term's quizzes. To a extent redundant with an earlier link.
