I was impressed with the way that Spartan helped students visualize molecules in three dimensions. A certain number of students seem to be able to get through the first semester of organic chemistry without making a good connection between three dimensional physical models and two dimensional formulas. Years ago, students were often exposed to mechanical drawing and solid geometry before they took organic chemistry. This suggested that, if you consider the percentage of chemistry majors in introductory and organic chemistry, it might be important to teach three dimensional visualization to students in freshman chemistry, particularly if the growing importance of this concept in biology and biochemistry is factored in. The molecular modeling capabilities of a program like Spartan are very useful in teaching students to visualize molecules in three dimensions. The ability to rotate the representation of a molecule under mouse or keyboard control helps students build a mental model of a molecule. It also helps students to move between models and three dimensional structures. These skills are useful to any student who will go on into biochemistry.

Chemistry majors need to learn to think like organic chemists. An important part of a chemist's mental picture of a molecule is an idea of the distribution of charge over the molecule. A **calculated** distribution of charge, clearly identified as such, can become an important part of a student's mental picture of a molecule. Both a mental picture of charge distribution and a calculated distribution of charge can be used to predict reactivity. The idea that computational chemistry is most valuable when it is used to predict an observable result is important. It gives students some idea of the validity, or lack thereof, of their computations. Spartan is a very fast computational package on current microcomputers; this suggests that the program can be very useful in the introductory organic course. The idea of making Spartan available to laboratory students who are waiting for one reason or another is an attractive one. Computations can be set up, submitted, and the results examined at separate times. Since computations run in the background, other students can use the program while computations are running.

I found the tutorials in the MacSpartan manual to be superb. After a brief demonstration of the capabilities of Spartan, organic students at either level quickly learned how to use Spartan as a computational package, with very little effort on my part. They were able to make the jump to applying the package to molecules that they were interested in with little or no hesitation. The ability to compute geometry, electron distribution, and even transition state geometry, allows students to ask all kinds of questions relevant to the understanding of organic chemistry. In fact, Spartan proved to be a very useful tool to get students to think like organic chemists.

Due to an institutional decision to phase out Macintosh computers, we are using PCSpartan this year. Wavefunction allowed us to upgrade our copies of MacSpartan to PCSpartan at a very reasonable fee (after return of the Macintosh hardware lock). We are running PCSpartan under Windows 95, on a TCP-IP network with a Windows NT server. So far, we have had no problems with the PC hardware lock.

CCCE National Workshops
Donald Rosenthal
<ROSEN@CLVM.CLARKSON.EDU>
Clarkson University

CCCE NATIONAL COMPUTER WORKSHOPS

Sponsored by the ACS Division of Chemical Education's Committee on Computers in Chemical Education (CCCE)

August 7 to August 9, 1998 (Just Prior to BCCE) at the University of Waterloo Waterloo, ON, Canada

The following workshops will be offered: (the title is followed by the name of workshop organizer)

A. INSTRUCTIONAL SOFTWARE FOR GENERAL AND ORGANIC CHEMISTRY What's Out There and How Are People Using It? Marco Molinaro (University of California, Berkeley)

B. USING THE WORLD WIDE WEB IN CHEMISTRY COURSES Brian Tissue (V.P.I. and State University)

C. DEVELOPING MULTIMEDIA MATERIALS FOR CHEMISTRY INSTRUCTION Charles Abrams (Beloit College)

D. PREDICTION OF PHYSICAL AND CHEMICAL

PROPERTIES BY COMPUTATIONAL CHEMISTRY Paul M. Lahti (University of Massachusetts, Amherst)

Descriptions of the workshops are presented below.

Each participant will register for one workshop which will schedule morning, afternoon and evening sessions on Friday, August 7 and Saturday, August 8 and morning and afternoon sessions on Sunday, August 9. The workshops will include both lectures and hands-on sessions. The registration fee is $ 120 Canadian (about $ 85 U.S.) before June 1, 1998 and $ 160 Canadian (about $ 115 U.S.) after June 1, 1998. The number of participants in each workshop is limited. Registrants will be accepted in the order received.

Information about the CCCE National Computer Workshops is available:

* by sending the message: SUBSCRIBE WORKSHOP your-name to: listserv@clvm.clarkson.edu

* on the World Wide Web under "Pre-Conference Workshops" (http://sciborg.uwaterloo.ca/bcce)

* by contacting the CCCE National Computer Workshops Director:

Donald Rosenthal Department of Chemistry
Clarkson University
Potsdam, NY 13699-5810
rosen@clvm.clarkson.edu
Telephone: (315) 265-9242

WORKSHOP DESCRIPTIONS

A. INSTRUCTIONAL SOFTWARE FOR GENERAL AND ORGANIC CHEMISTRY - What's Out There and How Are People Using It?
Marco Molinaro, MultiCHEM - Director of Multimedia Development, Department of Chemistry, University of California,Berkeley CA 94720 molinaro@cchem.berkeley.edu - http://mc2.cchem.berkeley.edu

The amount of chemistry instructional software is increasing exponentially. The purpose of this workshop is to:
1) expose you to what is out there,
2) give you hands-on experience with the software, and
3) learn how others are using the software in the classroom, in the laboratory, and as take home work for the students.

We will take time to explore, critique, and discuss some material in depth from both the CD-ROM and the World Wide Web realms with the goal that everyone interested will leave with a clear plan for implementing appropriate technology in their classroom.

The software we will focus on will be both Macintosh and Windows compatible. Some Macintosh- or Windows-only software will be mentioned for completeness.

B. USING THE WORLD WIDE WEB IN CHEMISTRY COURSES Brian Tissue, Department of Chemistry, V.P.I. and State University, Blacksburg VA 24061 - tissue@vt.edu
http://www.chem.vt.edu/chem-ed/workshop/

In this course participants will learn how to find, create, and use Web resources for their courses. We will begin by demonstrating and discussing what is available on the Internet. Participants will create basic HTML pages and FTP them to a server, and then progress to incorporating images, image maps, forms, JavaScripts, or other interactive elements into their pages. Discussions will focus on which Internet-based methods are best for different educational tasks. Participants should bring ideas and materials from which to develop Web pages. Either Macintosh or PC platforms may be used.

C. DEVELOPING MULTIMEDIA MATERIALS FOR CHEMISTRY INSTRUCTION
Charles Abrams, Department of Chemistry, Beloit College, Beloit WI 53511 - Abrams@Beloit.edu

Multimedia authoring is not as costly or difficult as it used to be. This workshop will introduce participants to several multimedia authoring tools and techiques, ultimately focussing on MacroMedia Director. Instructors interested in creating their own multimedia presentations, or helping their students do so, are especially encouraged to attend. We will learn how to take advantage of unique capabilities of computerized instruction (interactivity, visualization, etc.) that cannot be duplicated by other instructional media. Incorporating multimedia elements into web pages (using Macromedia's Shockwave) will also be covered.

No prior programming or graphics experience is required. By the end of the workshop, participants will have developed a short multimedia tutorial on a topic from general or organic chemistry, with the help of graphics and templates provided.

Macintosh computers will be used. However, the skills learned and all the software used is available and readily transferable to the Windows platform.

D. PREDICTION OF PHYSICAL AND CHEMICAL PROPERTIES BY COMPUTATIONAL CHEMISTRY

Paul M. Lahti, University of Massachusetts, Amherst MA 01003-4510 - lahti@chem.umass.edu

This workshop will be a hands-on session aimed at demonstrating and testing computational chemistry methods for the prediction of molecular properties. A survey of various force field, semiempirical molecular orbital, and ab initio molecular orbital methods will be made with consideration of their capabilities of predicting specific properties. Case studies will be carried out to evaluate properties such as: molecular geometry, conformational analysis, vibrational spectroscopy, UV-vis spectroscopy, dipole moments, and chemical reactivity. Time will be allotted for free-format labs when workshop attendees focus on problems of their own specific interest. Problems both of educational and research interest are encouraged. Extrapolation from molecular to macromolecular properties will be briefly considered, but generally will be outside the scope of this workshop.

Because of the applied nature of this workshop, some previous experience with computational modeling techniques will be expected. A brief overview of the methods used in the workshop will be given to orient workshop attendees sufficiently to proceed with the specific exercises given.

Pharmaceuticals, Their Discovery, Regulation and Manufacture OLCC-3

Jim Beard,
Catawba College
Salisbury, NC 28144
jbeard@catawba.edu

This is an invitation to register your school for the On-Line Chemistry Course for Upper Division Chemistry Students (Prerequisite - one year of organic chemistry) to be held during the Fall term of 1998. The on-line activities will be scheduled for September 14 to November 25, 1998. The title of the course will be "Pharmaceuticals, Their Discovery, Regulation and Manufacture." The course is sponsored by the American Chemical Society, Division of Chemical Education's Committee on Computers in Chemical Education (CCCE). In this course, the Internet will be used for discussions among students (student Listserv and WebBoard), faculty (faculty Listserv and WebBoard) and experts, all from around the world.

TOPICS MAY INCLUDE BUT ARE NOT NECESSARILY LIMITED TO:

1. Drug discovery including computer-aided design, combinatorial chemistry and other, earlier strategies

2. Development of clinically useable drugs including optimization of novel lead structures and assessment of pharmacodynamics, safety and efficacy of promising drug candidates

3. "Case studies" of the development and use of certain classes of widely used drugs including analgesics, antidepressants, anti-inflammatory drugs, antibiotics, AIDS and anti-cancer compounds

4. The FDA approval and FDA regulated testing process

PROCESS AND CONTENT RELATED GOALS OF THE PHARMACEUTICALS COURSE:

1. To provide an opportunity for students to investigate frequently used processes for discovery and manufacture of pharmaceuticals used as drugs for man and other animals

2. To provide the opportunity for students to gain an understanding of the general procedures for drug testing, its limitations, analysis, use and regulation

3. To provide an electronic forum which permits students to interact with professionals who are involved with the processes in 1 and 2

4. To provide an environment in which students will