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Computers in Chemistry

Enhancing Instruction in Upper Division Chemistry at California State University Fullerton

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Our active learning instructional computer facility has become a model for ongoing university-wide reform efforts….

At California State University Fullerton the Departments of Chemistry and Biochemistry and Physics have jointly established an active learning instructional computer facility where students explore models and data in the upper division chemistry and physics curricula. This facility is also a component of the larger W.M. Keck Foundation Center for Molecular Structure (CMolS), a core research and education center where faculty and students throughout the California State University system have the opportunity for joint research and teaching activities directed at the determination and critical analysis of molecular structures. An array of Silicon Graphics® workstations and a server housed in an "electronic classroom" provides a networking medium linking students and faculty across our

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curricula to resources and courses with common themes, but traditionally segregated. Through team teaching and utilization of resources and expertise across subdisciplines and disciplines, we are creating a learning pathway that coherently exposes our students in chemistry and biochemistry to more sophisticated problems and exploration. Computers provide visual reinforcement and interpretation for concepts and principles that students may have difficulty understanding and that cannot be treated easily or well by the problem-solving methodology. Our students have responded enthusiastically to the electronic classroom, and introduction of chemical computation into the curriculum has had a positive pedagogical impact.

Introduction

Instruction in the physical sciences is commonly carried out using the "problem-solving" methodology. Students are presented classical examples that illustrate the applicability of the subject, and they are expected to master the mechanics or algorithms of these examples and to be able to recognize new or unfamiliar situations where these skills can be applied. This works for some, but not all, students [1, 2], and it is essentially a passive learning mode [3]. Moreover, such an instructional process is rather different from the actual practice of the disciplines. Practitioners of science spend a great deal of time dealing with data, analyzing it, searching for connections within it, and representing it in different ways to better understand it. They also spend time examining physical and symbolic models to understand their applicability and limitations and to extract further information.

At California State University, Fullerton the Departments of Chemistry and Biochemistry and Physics have jointly established an active learning instructional computer facility. This facility is housed in a remodeled classroom equipped with ten Silicon Graphics workstations and a state-of-the-art Challenge L[1] server, networked together and to the campus internet backbone. This provides a networking medium linking students and faculty across our curricula to resources and courses with common themes, but traditionally segregated. This facility is also a component of the larger W.M. Keck Foundation Center for Molecular Structure (CMolS), a core research and education center where faculty and students throughout the California

[1] Challenge L is a trademark of Silicon Graphics, Inc.

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State University system have the opportunity for joint research and teaching activities directed at the determination and critical analysis of molecular structures.

The active learning instructional computer facility is used by students to explore models and data in the upper-division chemistry and physics curricula. The goals of this facility are:

- to develop course models that build on the basic science shared by the two disciplines, (This cooperative endeavor will lead to synergy among courses in the same discipline, and also between disciplines.)
- to replace portions of lecture time with exploration of data and models, (Sets of data and models will be organized to illustrate important concepts and principles that cannot be treated easily or well by the problem-solving methodology.)
- to systematically introduce students to exploration activities that utilize various computer applications, (Students will explore pre-prepared files during class under direct guidance of instructors. With experience students will create their own individually assigned or suggested work product, applying what they have learned to more sophisticated problems and exploration. Eventually they will move to free form assignments that allow them to explore specific content in detail and to test limitations of the theory and of the applications. As students proceed through the curriculum, their experience with applications will better prepare them for subsequent courses.)

A brief overview of some of the exploration activities and computer applications related to the chemistry curriculum and their use in this “electronic classroom” is presented in this article. Future articles will address each course and its activities in detail.

Exploration Activities and Computer Applications in the Upper Division Chemistry Curriculum

Introduction to Chemical Computation

CHEM210 is a new one-semester, two-unit sophomore-level course, “Introduction to

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Chemical Computation," which has replaced the computer programming course requirement in our major. Prior to 1993 our students were required to complete a course in elementary computer programming for their degree. We found, however, that the students were not transferring the skills learned to the chemistry curriculum. In CHEM210 students learn how to use various software packages while, at the same time, learning how to develop a logical sequence of steps towards solving a chemical problem or investigating a molecular system. This team-taught course introduces students to computers as tools to solve real chemistry problems. The faculty who teach the course are knowledgeable in all aspects of the course, but each teaches that portion of the course that falls in their area of expertise (e.g.; molecular modeling, Mathematica). The prerequisite for CHEM210 is one year of general chemistry, and it is assumed that students have some basic knowledge of word processing. In CHEM210 our students learn the fundamentals of operating systems (DOS, MAC-OS, UNIX[2]), data transfer (telnet, ftp, e-mail), navigating the Internet (Netscape), html (Web Wizard, asWedit), software for molecular modeling and chemical computation (Spartan[3], RasMol[4]), mathematical manipulation (MS-Excel[5], Mathematica[6]), presentation development (PowerPoint) and, several electronic library resources. The focus is on chemical applications. Students are not required to purchase software or computer time other than a campus-wide computer lab fee card. Formal lectures are not used. A complete description of the course, including syllabus, assignments, instructions, and an archive of student homepages may be found at http://zeppo. fullerton.edu:8080/~sharding/ 210syl.html.

All assignments in CHEM210 are exchanged electronically. Students post graphical results and the results of their database searches on their personal homepage. Using Powerpoint, students are introduced to the basic elements of visual design, content selection and creation, and importing and exporting of graphic images. Web authoring software allows them to create their individual homepages. Students are introduced to the chemical literature in two online sessions. They first learn to access scientific information freely available through the internet at several sites such as the

[2] UNIX is a registered trademark of UNIX System Laboratories, Inc.
[3] Spartan is a trademark of Wavefunction, Inc.
[4] RasMol v2.5, Molecular Visualization Program by Roger Sayle, Copyright, 1994, Glaxo-Wellcome.
[5] MS-Excel is a registered trademark of Microsoft Corporation.
[6] Mathematica is a registered trademark of Wolfram Research, Inc.

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ChemCenter page http://www.chemcenter.org) at The American Chemical Society's web site. They then learn to access resources available through our library's computer system and internet connection, which has special access privileges to several scientific subscription databases.

The level of presentation in the molecular modeling portion of CHEM210 is aimed at students who have taken or who have recently finished at least one semester of organic, but who have not yet taken physical chemistry. Students meet for two interactive sessions with Spartan and one with RasMol. Background presentation begins with a discussion of why chemists use models and the flaws associated with static models commonly used by students. The background discussion includes some molecular orbital theory but avoids detailed quantum mechanics. Problem sets are written and frequently revised to emphasize certain chemical concepts, demonstrate various features of Spartan and molecular modeling in general, and introduce a small amount of new chemistry. Later in the course, students search the Brookhaven Protein Data Bank (http://pdb.pdb.bnl.gov) via Netscape and select and download a structure, which they then manipulate with Rasmol. A gif file of the final structure, along with a brief explanation, is emailed to the instructor. Many students choose also to include this structure on their home page.

The goal of the mathematical manipulation portion of the course is not to teach the students computer programming per se. Rather, the students learn how to use spreadsheets and symbolic algebra software while, at the same time, learning how to develop a logical sequence of steps towards solving a chemical problem or investigating a molecular system. The students meet for two interactive lectures on the use of MS-Excel. Students are introduced first to spreadsheet data entry, cell formatting, and basic mathematical calculations, including the built-in functions that are commonly employed in the sciences. These are followed by more sophisticated techniques, such as graphing, linear regression, and construction of a searchable, linkable database (the periodic table). The problems that the students are asked to solve are presented to them in increasing level of sophistication and difficulty. These problems help them to master the use of the spreadsheet while, at the same time, they learn how to develop a logical sequence of steps towards solving chemical problems. Later in the course, students are introduced to very basic Mathematica scripting in one interactive session. They learn how to construct a simple instruction, do a repetitive calculation, produce two- and three-dimensional graphs, and manipulate arrays.

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Organic Chemistry

CHEM301 and CHEM305 are the organic chemistry courses for biochemistry and chemistry majors respectively. Here, molecular modeling and quantum mechanical calculations are used to illustrate and explore various topics in laboratory and lecture. Exercises using the Spartan computational package [4, 5] have been designed with significant focus on introduction and reinforcement of chemical concepts from lecture and laboratory and prediction of chemical properties and reactivity. Included in these exercises are studies on cation and radical stabilities, S_N1 and S_N2 transition states, resonance theory, molecular geometry and dynamics, and strain theory. Some of these exercises may be found at http://zeppo.fullerton.edu:8080/~sharding/chem301bsyl .html.

Inorganic Chemistry

In the inorganic chemistry laboratory, CHEM325L, molecular modeling using the Spartan computational package has been used to examine physical properties of various products of synthesis. For example, Silly Putty™, an elastic polysiloxane, is prepared from dichlorodimethylsilane. Students also prepare the diphenyl analog and discover it to be a crystalline solid, dubbed “Serious Putty”. Molecular modeling reveals the reason for this difference. Calculations on a short strand of the polymers shows that the methyl groups of Silly Putty are sufficiently far apart to move past one another with relative ease, while the phenyl groups of “Serious Putty” suffer serious impairment of motion.

Physical Chemistry

The topics covered in physical chemistry for biochemistry majors, CHEM361A/B, include classical thermodynamics, solutions (ideal and real), phase changes, kinetics, statistical mechanics, quantum mechanics, chemical bonding, spectroscopy, symmetry, and x-ray diffraction. The emphasis is on biochemical applications. Exercises using the Spartan computational package have been designed to illustrate important concepts in chemical bonding and spectroscopy. The molecular models are revisited during discussions on symmetry. Students build energy-minimized models of small molecules and molecular ions, then calculate and visualize various quantum concepts and properties of the system, such as wave functions, molecular orbitals, and charge density. At first, these tasks are completed in a somewhat transparent fashion, allowing the program to set default parameters. Later, students explore the effects of varying parameters and explaining the changes they observe. Students then use the molecular

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models they have already built to calculate normal mode vibrations, animate them (with far greater clarity that the instructor using projections and arrows on the board), and they note changes in dipole moment and polarizability. Because organic chemistry is a prerequisite for physical chemistry, we expect that not only should students have a working knowledge of Spartan, but that they would be able to correlate the quantum mechanical treatments with their prior explorations in organic chemistry. Mathematica [6] notebooks have been created that allow students to explore partition functions in statistical mechanics and quantum mechanical models of the particle-in a box and the harmonic oscillator. Examples of these exploration activities may be found at http://zeppo.fullerton.edu:8080/~kkant/chem361.html.

PHYS455 is a course in quantum mechanics for both physics and chemistry majors that emphasizes atomic and molecular structure, transitions and reactions. It is based on the book, *Quantum Methods with Mathematica* [7]. Here, Mathematica is used to show three-dimensional plots of the spherical harmonics and evaluate normalization integrals for hydrogen. A harmonic oscillator project allows students to explore the correspondence principle by making comparisons between the position probability density for a classical harmonic oscillator and a quantum harmonic oscillator. Some of the animations created with Mathematica may be found at http://chaos.fullerton.edu /~heidi/anim.html.

CHEM543 is a graduate course in physical biochemistry. This course examines the nature of macromolecular structure and physical methods for structure determination and analysis, including spectroscopy, multidimensional nuclear magnetic resonance and x-ray diffraction. Using the Biosym suite of programs InsightII/Biopolymer/ Homology, students examine amino acid sequences for homology, predict secondary structure, display three-dimensional structures, and predict tertiary structure. Students study the structural relationship between apparently disparate molecules and speculate as to the events and processes of evolution at the molecular level. Diffraction data obtained either from CMolS or the Brookhaven Databank is manipulated and analyzed with XtalView[7]. Students calculate and display Patterson functions and electron density maps.

[7] XtalView, Release 3.0 by Duncan E. McCree , Copyright, 1995, The Scripps Research Institute.

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Biochemistry

Molecular modeling applications are quite useful in describing the structure of macromolecules. Relevant aspects such as surfaces, charge density, and accessible volume can be demonstrated and discussed, giving the molecule a concrete individuality not attainable from text or lecture alone. Programs such as Biosym's InsightII and Discover have already seen limited use in our upper division biochemistry lecture course, CHEM 423A/B. We plan to focus lectures on stereochemistry, protein secondary and supersecondary structure, tertiary structure, quaternary structure, as well as polysaccharide and nucleic acid structures. Further applications can easily be used to visualize the solvent accessible surface and electrostatic surface of proteins, which will aid students' understanding of the binding of substrates and the mechanism of action of enzymes. Student projects will involve answering questions about various levels of structure of a protein, including questions that concern site-directed mutagenesis. Students will study the structural relationship between apparently disparate enzymes, speculate as to the events and processes of evolution at the molecular level, and, thus, be able to better explore and conceptualize the relationship between structure, enzyme kinetics, and mechanism. Similar exercises can vitalize the study of tRNA structure, the difference between "B" and "Z" DNA (believed to be of importance in the regulation of gene expression), the molecular basis of antibody-antigen interaction, and the structure and surface properties of viruses.

Computing Facilities

The active learning instructional computer facility is housed in McCarthy Hall of Letters and Science. The facility, which can double as an "electronic classroom," provides faculty and students access to 10 Silicon Graphics 100 MHz Indigo R4400 PCs, each with 32 MB memory and 0.5 GB system disk networked to a Challenge L server. The server is configured with two 75 MHz TFP CPUs, 256 MB memory, and 12 GB of system disk storage. The computer array is completed by an Indigo2 150 MHz R8000 Extreme with 64 MB memory and 2 + 4GB in system disks, located in the x-ray diffraction laboratory. The entire array is networked by Ethernet TCP/IP.

The facility is maintained by a full-time department instrumentation and software support technician. A staff scientist at CMolS and postdoctoral fellow also provide system support. Technical staff are essential for efficient operation of the facility and timely delivery of computational resources. During the academic year, the facility is

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open 35 hours per week for student use, except when booked for formal classroom activities. Students are issued accounts when they enroll in a specific course. Six student assistants from the Departments of Chemistry and Biochemistry and Physics support the facility by helping students with software applications and projects, answering technical questions, and maintaining security (http://zeppo.fullerton.edu: 8080/~kkant /sgischs97.html).

Software available includes an assortment of molecular modeling and refinement modules, sequence and homology searching modules, and solids and polymer building modules from Biosym Technologies, Spartan, Hyperchem, RasMol, Mathematica, Gaussian94, O[8] and X-PLOR[9]. San Diego State University, which is the home of the first core facility in the California State University system, the Microchemical Core Facility, maintains the GCG software package for DNA and protein sequence analysis with GENBANK database. This software is available through the CSUNET.

Discussion

It has taken more than two years to enhance the curriculum as described in this article, with several previous years of pilot studies. Computer use in the curriculum should be integrated universally, albeit to varying degrees, but this integration should be gradual until it naturally follows from one course to the next. To have an impact on the curriculum, the activities developed should form a significant comprehensive component of the course and not appear to the students as a collection of unrelated exercises on isolated topics. The transition for both students and faculty to use computers as tools for teaching and learning must be relatively easy to be effective, so that students can focus on the content of the activities in which they are actively engaged, faculty can make assignments and monitor progress of students, and neither is bogged down by having to learn much about the idiosyncrasies of the hardware. Other courses at the college level are designed to teach more sophisticated computer programming and system operations. We do find, however, that each semester students in our courses seem more computer savvy and less anxious about using computers than the previous semester's group.

[8] O, A General Purpose Macromolecular Modelling Environment by T. Alwyn Jones and Morten Kjeldgaard, Copyright, 1993, Uppsala University.
[9] X-PLOR v3.1, A System for X-ray Crystallography and NMR by Axel T. Brunger, Copyright, 1992, The Howard Hughes Medical Institute, Yale University.

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Our students have responded to the electronic classroom with great enthusiasm. With modest guidance and supervision, students learn to use applications and, in fact, become reasonably sophisticated users quite quickly. They devour the manuals with greater alacrity than do faculty, they help each other out, and they desire to do more. Computers provide visual reinforcement or interpretation for concepts and principles that students may have difficulty understanding and that cannot be treated easily or well by the problem-solving methodology. Student surveys at the end of each semester help instructors to make appropriate modifications to exercises, problems, and projects, removing those that the students find confusing or that the instructors find to be of little value and introducing new ones that reinforce student learning and challenge then to explore, to function as practitioners of science. Student assistants, if chosen carefully, are an excellent source of support. They learn by teaching others and acquire invaluable skills.

Our approach of team-teaching and utilization of resources and expertise across subdisciplines and disciplines has been a good one, and introduction of chemical computation into the curriculum has had a positive pedagogical impact. Students benefit from instruction by those faculty whose expertise is with particular computer applications, and involved faculty benefit from creative discussion as exploration activities are developed and evaluated. We continue to work to better correlate courses within our discipline and across disciplines. Steps are being taken to coordinate joint chemistry/physics courses in computational methods, quantum physics, and thermodynamics. As we build on these correlations, and our students progress through their upper division courses, we are creating a learning pathway that coherently exposes our students to more sophisticated problems and exploration. Using computational tools, they will begin to see the interconnections among topics in chemistry and physics and learn how these topics can be viewed and described from different perspectives. We have already transferred to the high school level, with very favorable results, several of the enhancements to the curricula that utilize molecular modeling and mathematical manipulation. Our active learning instructional computer facility has become a model for ongoing university wide reform efforts towards better overlap among course offerings across curricula and engaging students by means of distance learning.

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