ELECTRONIC CLASSROOMS

Wilmon B. Chipman
Dept. of Chemical Science
Bridgewater State College
Bridgewater, MA 02325
CHIPMAN@TOPCAT.bsc.mass.edu

Chemistry is probably the best discipline which could be taught in an electronic classroom. There are two reasons for this - the nature of the material and the availability of software. Chemistry is complex, abstract, and often needs to be visualized in three dimensions. In organic chemistry and biochemistry more than one level of visualization may be essential for understanding. There are many excellent molecular modeling programs that can supplement the normal array of animation and authoring programs.

As a part of the design of the J. Joseph Moakley Center for the Application of Technology which is being constructed at Bridgewater State College, we have examined existing electronic classrooms at a variety of colleges and universities in the northeastern United States. As a result of this study, we have identified the following categories of electronic classrooms:

1. the two microcomputer classroom. Although there is no reason why only one microcomputer cannot be used, the use of a high level Macintosh **and** a 486 IBM/ clone allows full access to a larger base of software. A computer projection device, which may vary from a LCD panel on an overhead projector to a sophisticated video projection system, completes this model. We were surprised to find that departments which could afford more sophisticated setups often chose this model.

2. the desktop microcomputer model. The addition of ten to thirty microcomputers and a local area network (LAN) which is often connected to the institutional backbone, converts the two-microcomputer classroom into this model. A number of colleges have found that two students per microcomputer works better than one; hence fifteen is a popular number for student stations. It is essential that such a classroom be tiered so that the computer monitors do not interfere with the view of the projection TV screen. Although one would think that this type of classroom could be used as a computer laboratory (if adequate security is provided), many institutions found that interest in using the electronic classroom as a classroom did not leave much time for student use outside of class.

3. the maximalist model. The addition of screen control and screen sharing from a "master" microcomputer is relatively easy to implement in software. Some faculty object to the "control" implications of this model; others like the software control system.

4. the workstation model. At least one university in the northeast has an electronic classroom that uses UNIX workstations. The decreasing cost and increasing power of workstations may make this the choice of the future. An easy to use graphics user interface (GUI) can hide the complexities of the UNIX operating system and provide Macintosh-like ease of operation. If such a system is networked properly it can provide enormous computing power at very reasonable cost.

EDITOR: Bill is willing to set up a bulletin board about electronic classrooms at his college. Please send any suggestions for the format and other subjects of interest to Bill. This sounds like a great idea for getting ideas for those of us who are in the process of introducing electronic classrooms to our colleges.

HyperChem for Windows, Release 2. Reviewed by: **Andrew N. Welch and Yuzhuo Li**, Clarkson University, Potsdam, NY 13699. E-mail: welchan@craft.camp.clarkson.edu

Autodesk, Inc.: Scientific Modeling Division, 2320 Marinship Way, Sausalito, CA 94965. List Price $3500; educational discount price $595.

HyperChem for Windows is a powerful molecular modeling program that performs calculations using *ab initio* and semi-empirical quantum mechanical methods. HyperChem is designed in such a way that all of its commands and output can be controlled externally by other Windows programs, such as Excel or Visual Basic. In order to run HyperChem, the following is required: an IBM-PC compatible computer with an 80386 CPU and an 80387 math coprocessor, or an 80486 or higher CPU, 4 megabytes of memory, a hard disk with at least 5 megabytes free, a VGA or better video display, a parallel port for the locked version, a pointing device compatible with Windows 3.0 (such as a mouse), MS-DOS Version 3.1 or higher, and Windows 3.0 or higher.

HyperChem was tested on both a 486-25 and a 386-33. Installation was quick and easy and was completed in under ten minutes. There are two versions of HyperChem, an unlocked version and a locked version. The unlocked rendition requires no special action. However, the locked version demands that a hardware key be continually present in the parallel port. This form of copy protection does not permit simultaneous use of the software on different machines.

Upon loading HyperChem, the screen resembles that of other Windows programs. There are pull down menus, buttons for moving and scaling both the molecule as well as the entire HyperChem win-

dow, and the blank workspace.

Drawing molecules in HyperChem is uncomplicated. A default atom is first selected then bonds are drawn to form a skeletal structure. The default atom is selected by double clicking an icon and then using scroll bars to select an element. Atom charge and constraint of atomic geometry, bond length, angle and torsion angle can all be specified. The angle as well as stereochemical conformations, such as *cis-* or *gauche-*, can be specified. For a biochemist, databases of standard amino acid residues and nucleic acid residues can be employed to make macromolecules. A user selects the conformation and presses buttons labeled with residues to make a molecule. Zwitterions and counter ions can be specified. Once a molecule is created, a residue can be treated as a unit. It is not difficult to mutate a specific residue.

Once a molecule is drawn, a user typically invokes the so-called Model Builder. This section of HyperChem changes the entered 2-D representation into a 3-D drawing. This feature makes it easy to spot errors in input and change them. On the 386-33 and 486-25, the Model Builder worked essentially instantaneously. Once the model is built, the user is able to use many of HyperChem's features.

The display of molecules is flexible. Color can be used; atom labels range from the common element name to its chirality and a residue can be displayed with its name and/or position. Hydrogen bonds can be displayed. There are five rendering options: sticks, dots, sticks and dots, spheres, and disks (a "flatter" version of the sphere). Sphere rendering was very quick compared with other molecular modeling programs. Several molecules may be displayed together, superimposed if desired, to show the differences between them, such as what is different between an optimized and an unoptimized molecule.

There are several different methods of selecting certain parts of a molecule. Atoms, residues, or entire molecules may be selected and manipulated as units. A sphere may be used to select objects encompassed in the 3-D area. There is a NOT operation that will select what is currently unselected, and that which was currently selected becomes deselected. Backbones, side chains, and rings may be selected without having to select each individual element. You can even extend a selection along a chain until you get to an sp^3 carbon atom. A group of selections may be named and used later. Additionally, certain selection names are used in changing the molecule. For example, if the PLANE selection is input, the user may carry out a molecular reflection across the plane. Selection is very well supported in HyperChem.

There are four molecular mechanical force fields available: MM+, AMBER, BIO+, and OPLS. In general, these methods are designed for macromolecules, nucleic acids and proteins. However, although MM+ was originally designed to be used with organic molecules, the scheme was modified to broaden its potential use. Dielectric interaction (epsilon) and nonbonded interactions can be scaled and changed from what they would normally be when the molecule is a gas. Geometry constraints for bond length, angle, and torsion angle are able to be defined. Semi-empirical methods available are Extended Hückel, CNDO, INDO, MINDO3, MNDO, and AM1. Options include convergence criteria, charge, spin multiplicity, spin pairing, electron excitation state, and the DIIS procedure which can accelerate convergence. For each method, there are tables of data that contain information such as ionization energy and Slater exponents; numbers come from values obtained in literature. These parameter tables may be edited and recompiled to fit special applications. A periodic box may also be specified to represent solvent effect. Geometry may be optimized by the steepest descent, Fletcher-Reeves, or Polak-Ribiere methods. Geometric optimization and single point calculations were compared with results obtained with the Gaussian 90 program running the same type of calculation, and the results were essentially the same. The speed of these calculations is not slow for a PC. Nitrobenzene was optimized in 36 seconds and azidoadamantine was optimized in 43 seconds. There appear to be no significant computational discrepancies between the two programs.

HyperChem, because of its integrated nature, deviates from the traditional method of log file output from calculation stages. Contour plots, superimposed on the molecule, can depict electrostatic potential, spin density, charge density, and orbital information. Molecular dynamics can be animated. A temperature routine can be used to monitor the effects of heating on the screen. Snapshots may be saved for later study. Additionally, there is a facility where graphs of different energies, such as kinetic and potential, may be plotted during the run.

There is a log file facility used to store commands. It is useful and flexible. Events are saved and the user may put comments into the file at will. Unfortunately, there is no facility for datafile conversion. This means that a user must write his own converter program if he wants molecules created in HyperChem to be used with external computational programs. The only filetypes supported are .HIN, which is the proprietary format, and .PDB, the Brookhaven Protein Data Base format. The documentation describes the use and the method of obtaining .PDB files. Pictures of the HyperChem workspace can be saved to the clipboard as a Windows Metafile (.WMF) or as a Windows Bitmap (.BMP). These pictures are easily inserted in other documents.

Probably the most useful aspect of HyperChem, and that which separates it from other pro-

grams, is its ability to be controlled externally by other programs. The tutorial provided describes using Excel to drive HyperChem. The torsion angle in hydrogen peroxide is changed by an Excel macro and the new energy is recomputed. Cells are automatically filled with the appropriate data and a graph can be plotted. There is considerable potential for user interaction in the program. A user is able to write routines in any language that is able to provide DDE (Dynamic Data Exchange) links to Windows. If desired, additional optimization or other kinds of manipulation of molecules is able to take place outside of HyperChem.

The online help is sufficient. There is a glossary that assists beginners in learning specific terms. Details on using the program's features are suitable. The documentation is superb. The tutorial does not take longer than a work day to complete and yet it illustrates most of HyperChem's capabilities. There is a guide for novices that explains much of the theory of computational chemistry. The language is comprehensible even to a beginning chemist. This guide explains which method and parameter set is best for each type of calculation. The reference guide is very complete and discusses not only program operation but also methods of interfacing HyperChem externally.

This program would be of considerable use to a first year chemistry, organic chemistry, biochemistry, or physical chemistry student. Because of the ability to show molecular geometry, concepts having to do with structure, bonding, interactions, and polarities become much easier to learn. The Windows platform allows the user to install many special devices that aid the learning process. For example, a projector can be used to show an entire classroom clearly what is on the computer monitor. These devices, sold by third party vendors, resemble overhead projectors that have a wire that connects to the computer.

Many students have difficulty visualizing the three dimensional shapes of molecules. With HyperChem, a large number of molecules may be drawn, optimized, and displayed on the screen. A lab could be designed where each student is assigned several molecules and asked to use Hyperchem to predict what the molecular shape would be. Different groups of students may be assigned different sets of molecules generating a larger database of structures. Students then would be able to deduce empirical rules on how to determine shape. Alternatively, the teacher may program the molecules and optimize them as a batch job with an external program. Then another program could be written that presents the data as a sort of "slide show." Students are then able to discover the correlations themselves and deduce the rules that determine molecular geometry. Another opportunity to use HyperChem for first-year students is when gases are studied. A sample of some gas may be heated and students can watch its effects on potential and kinetic energies and on the molecule itself. For the Organic Chemistry student, HyperChem can be very useful in teaching stereochemistry. It is easy to build molecules with different chirality, label each chiral atom, and rotate each to demonstrate the difference between the two molecules.

For more advanced students, the use of HyperChem can demonstrate the concepts of computational chemistry. Typically, one would have to use many programs to show differences between the different algorithms. However, because HyperChem has such a large array of methods, only one program needs to be learned. Additionally, the traditional text-based computational systems are ineffective in motivating students because the interface is more cumbersome to use.

In conclusion, HyperChem was found to be a very powerful tool. There is a new version that is currently in the process of being tested that includes several more computational methods including configuration interaction, better support for metals and inorganic compounds, more options for specifying stereochemistry, a floating element selection box, UV/VIS and vibrational analysis, and more extensive orbital analysis. HyperChem is quick, accurate, and, for the most part, easy to use. As an educational and research tool, the reviewers recommend this software.

THE COMPUTER CONFERENCE ON APPLICATIONS OF TECHNOLOGY IN TEACHING CHEMISTRY - THE FEBRUARY TRIAL SESSION AND THE SUMMER CONFERENCE

by Donald Rosenthal, Department of Chemistry, Clarkson University, Potsdam NY 13699 (ROSEN@CLVM.BITNET)

and **Thomas O'Haver**, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742 (TO2@UMAIL.UMD.EDU)

INTRODUCTION

The summer computer conference is the first such conference sponsored by the Division of Chemical Education's Committee on Computers in Chemical Education. Articles on the summer Computer Conference and Computer Conferencing appeared in the Fall 1992 issue of this Newsletter.