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.

We view this conference as an experiment and have tried to design the format to take advantage of the unique features of computer conferencing. We decided to test the format and other aspects of the computer conference by scheduling a trial session during February. The purpose of the trial session was to determine how well the proposed format worked and to obtain feedback from participants which might be used to modify the format and instructions to participants and authors. PRE-TRIAL ACTIVITIES

Upon registration for CHEMCONF ten pages of INSTRUCTIONS FOR PARTICIPANTS were sent to each participant. Twelve pages of INSTRUCTIONS FOR AUTHORS were sent to each author. Just prior to beginning the trial session there were over two hundred registrants from twenty-four countries.

Three papers were selected for the trial session:
Paper 1: "How to Make Computer-Assisted Instruction Fail" by Stephen K. Lower, Simon Fraser University, Canada (three pages),

Paper 2: "Windows and Networks: Lowering the Activation Energy for a Chemistry Department Microcomputer Facility" by Thomas O'Haver (eight pages),

Paper 3: "Some Computer Graphics Examples" by Thomas O'Haver (seven pages plus twenty-five figures each converted and transmitted as a separate text file).

These three papers were selected because each was quite different from the other. Paper 1 was similar to a paper which Professor Lower distributed at the 12th Biennial Conference on Chemical Education at UC Davis last summer. Paper 2 appeared in the Fall 1992 issue of this Newsletter. Paper 3 was prepared specifically for the trial session and was designed to provide participants with examples of graphics and to provide practice in downloading and viewing figures.

Prior to the beginning of the trial session the abstracts of the three papers were distributed. The trial session schedule was sent out a few days before the beginning of the session. TRIAL SESSION.

The papers and figures were distributed on Monday, February 1. Each paper contained questions intended to stimulate discussion by the participants. Short questions were sent by participants to the authors or to other participants during the next three days, i.e. questions for Paper 1 were sent on Tuesday, questions for Paper 2 were sent on Wednesday and questions for Paper 3 were sent on Thursday. In the second and third week two days were devoted to the discussion of each paper. The authors answered short questions directed to them at the beginning of the discussion of their paper. An evaluation form was distributed on February 16 and was to be returned to Thomas O'Haver via electronic mail before the end of February.

How well did the trial session and the proposed format work? Participants were generally enthusiatic. There were some problems. These will be discussed later. The following are some of the comments received:

* Great conference... I hope more are in my future. Mike Whitbeck, University of Nevada at Reno
* So far I have enjoyed the discussion and also learned a lot. It is great. Angelo R. Fernando, University of Alberta
* ... many (messages) are immensely helpful and thoughtful. Allan Smith, Drexel University
* We're all operating . . on the cutting edge of a new form of information and idea exchange. Carl H. Snyder, University of Miami
* I've learned and had fun. Paul Edwards, Edinboro University of Pennsylvania
* It feels like a real conference. You get snippets of conversations and ideas which add up to a coherent whole after some time. Dan Bearden, Clemson University
* I have found this trial session at once informative, energizing mind-boggling, fascinating and a tremendous source of ideas. The mind-boggling fascination is, that from the computer in my office, I am in contact with people all over the world -- doing exactly the same thing I am. ... a chance to learn, a chance to share new information. Elisabeth T. Kintner, University of Pittsburgh - Johnstown
* ... the excitement of developing ideas, clarifying points, getting to the position where I better understand what should happen in my classes ... Charles Sundin, University of Wisconsin - Platteville
* I think it has the potential for making us all feel a little less isolated. Robert Brown, Douglas College, Canada
* There was ample time for discussion. Papers and discussion could be examined in a leisurely manner. Participants were able to ask short questions of authors and obtain well thought out answers. Donald Rosenthal, Clarkson University
* . . thoughtful responses (keyboard is better than just discussing, since you do have to think . . about what you are writing.) Frank Darrow, Ithaca College
* Allowed everyone to have a voice. Doug Williams, Kalamazoo College
* The entire concept was wonderful. Opens new horizons. Howard Dess, Rutgers University .

One question that was asked on the evaluation form was "What did you like most about the Computer Conference?" Some of the above comments were made in response to this question. Other comments occurred spontaneously during the trial session.

Considerable discussion was generated during the conference with

many of the registrants participating. One participant reported the trial session had generated over two hundred pages of print out. (This does not include 80 pages of evaluation from 34 participants.) The papers and full discussion are available and can be accessed via electronic mail. (If you are interested, contact Thomas O'Haver at T02@UMAIL.UMD.EDU.)

Participants were asked to provide an overall evaluation of the papers, discussion and meeting on a scale from 1 to 5 where 1 is poor, 3 is average and 5 is excellent. The overall evaluation of the papers ranged from 3 to 5 with an average of 3.7. The discussion was rated from 2 to 5 with an average of 3.5. The trial session was rated from 3 to 5 with an average of 4.1.

Paper 1 listed eleven things a teacher could do to make computer-assisted instruction (CAI) fail. The paper was written in an ironic style and generated the most wide-ranging discussion, including the use of CAI, simulation and the role of more traditional teaching methods in a course which uses CAI.

Paper 3 contained examples of black and white, gray scale and color graphics. Some participants identified difficulties in the transmission of graphics and offered solutions and suggestions for the better handling of graphics. Some participants didn't even try to work with the figures. This discussion was most useful. As a result, some modification in the instructions and in the handling of graphics will be made for the summer conference.

Another question which was asked on the evaluation form was "What did you like least about the conference?" Many of the responses to this question reinforced comments made during the session. Rather than listing individual comments, we will summarize some of the conclusions.

"Noise" was generated by some participants due to a lack of familiarity with electronic mail and LISTSERV, a lack of discipline on the part of some registrants and inadequate instructions. Some registrants when they discovered more about the nature of the trial session and the volume of mail it would generate decided to sign off CHEMCONF but did not know how to do it properly. We all received the message "I want out". A few other extraneous messages added "noise".

The first week was designed for SHORT QUESTIONS to the authors or participants. All such questions were to be sent to CHEMCONF so that all participants would know what questions the authors were being asked. Private messages were to be sent to the authors identifying grammatical or other errors, or messages to Tom O'Haver asking for technical assistance. Some participants used the first week to begin discussion. This was not our intention. The first week was to be used for reading the papers, asking short questions and preparing for the discussion.

Some participants introduced "noise" by discussing one paper during the time allocated for discussion of another paper. Another problem was that even though a specific two days was allocated to the discussion of a particular paper several threads of conversations intertwined. Even if the thread can be identified, the segments of the thread are not necessarily received sequentially. The labeling of the message was not always sufficient to identify the thread nor indicate where the message fit on the thread.

We sought to obtain information on the degree of participation by each registrant in the trial session. We consider this evaluation to be an important aspect of the trial session (and summer conference) experiment. Several registrants indicated that February was a busy time for them. When someone goes to a meeting the participant frequently makes a definite commitment to participate. We are interested in learning how much of a commitment of time and effort registrants will make to a conference which extends over TWO MONTHS in the summer. The results of the trial session survey indicated that those participants who returned the survey:

1. accessed the discussion from zero (only read the papers) to seventy times. The average was 24 times.
2. Devoted from 2.3 to 28 hours to the trial session. The average was 9.5 hours.

Those who participated in the evaluation process probably devoted more time to the trial session than the average registrant.

The trial session evaluation form contained the question: "What changes can be made to improve the computer conference?" Some suggestions were made during the trial session. Some of these suggestions have already been mentioned. The suggestions were not always consistent. Some participants wanted more structure, others wanted less. Some participants wanted more than two days devoted to discussion of each paper. Other participants were afraid that additional discussion time might result in too much discussion. If three papers generated 200 pages, will fifteen papers generate 1000 pages! Who wants to wade through so much discussion? There was an appeal for brevity in discussion. It is obvious that some participants are addicted to electronic mail. The suggestion was made that we impose voluntary limits on the number of times participants can submit discussion on any one paper. Registrants will need to exert more self-discipline and the conference manager may need to play a more active

role in managing the summer conference. In order to reduce the noise, the conference manager (Tom O'Haver) will announce the beginning and end of each session. This will avoid confusion associated with different time zones. Registrants will be asked to limit themselves to the designated activity, e.g. SHORT QUESTIONS for Paper 1 or DISCUSSION for Paper 2. Time for GENERAL DISCUSSION may be available on another LISTSERV or at other designated times. Discussion of papers will generally be for two days, but where discussion is scheduled for Friday and Monday the weekend will be available. This effectively provides four days.

Additional details will be provided for registrants just prior to the summer conference. SUMMER CONFERENCE - June 14 through August 20, 1993.

Abstracts for the following fifteen papers have been received and the tentative order of presentation is as indicated:
SESSION ONE

1. CULTURAL DIFFERENCES REFLECTED BY AN INTEGRATED MEDIA CHEMISTRY COURSE - AN AMERICAN/ISRAELI PERSPECTIVE. Nava Ben-Zvi, William S. Harwood, Ahuva Leopold, and Lisa L. Ragsdale Hebrew University, Israel and University of Maryland

2. FOR LANS SAKE: SUGGESTIONS FOR THE USE OF NETWORKED COMPUTERS IN CHEM ED B. James Hood, Middle Tennessee State Unversity

3. WHY DO ELECTRONS AND NUCLEI FORM ATOMS AND MOLECULES?: A GUIDED, INTERACTIVE EXPLORATION IN QUANTUM MECHANICS John P. Ranck, Elizabethtown College

4. THE USE OF COMPUTERS IN A JUNIOR-LEVEL ANALYTICAL CHEMISTRY -PHYSICAL CHEMISTRY LABORATORY COURSE Donald Rosenthal, Clarkson University

5. IT'S HOW YOU PLAY THE GAME: DESIGN OF AN ELECTRONIC ASSISTANT FOR ORGANIC QUALITATIVE ANALYSIS Joyce C. Brockwell, Northwestern University SESSION TWO

6. INDIVIDUAL COMPUTER-GENERATED GRAPHICAL PROBLEM SETS Frank M. Lanzafame, Monroe Community College

7. INTEGRATING COMPUTERS INTO THE HIGH SCHOOL CHEMISTRY CLASSROOM William J. Sondgerath, Harrison High School, West Lafayette, Indiana 8. USING THE AIRWAVES: A SATELLITE M. S. FOR INDUSTRIAL CHEMISTS. K. J.Schray, N.D. Heindel, J. E. Brown, and M. A. Kercsmar. Lehigh University

9. APPLICATIONS OF NETWORKED COMPUTERS AND ELECTRONIC MAIL IN A CHEMISTRY COURSE FOR NONSCIENCE STUDENTS Carl H. Snyder and James Shelley, University of Miami

10. COMPUTATIONAL CHEMISTRY AS A CENTRAL FEATURE IN THE TEACHING OF ORGANIC CHEMISTRY Joseph Casanova, California State University at Los Angeles SESSION THREE.

11. STAFF DEVELOPMENT IS THE BIGGEST COST IN COMPUTING David W. Brooks, University of Nebraska-Lincoln.

12. THE COMPUTER CO-OP: TEACHING ORGANIC CHEMISTRY ON A CONFERENCE IN AN INTERDISCIPLINARY MACINTOSH LAB Carolyn Sweeney Judd and Robert G. Ford, Central College, Houston Community College System.

13. FINITE DIFFERENCE SOLUTION OF THE DIFFUSION EQUATION ON A SPREADSHEET Douglas A. Coe, Montana College of Mineral Science and Technology.

14. CHEMULATE! A SIMULATOR OF UV/VIS KINETICS EXPERIMENTS FOR THE MACINTOSH Richard S. Moog, Franklin and Marshall College.

15. MENU DRIVEN PROGRAMMING FOR STUDENTS AND TEACHERS Reed Howald, Montana State University.

Those wishing to register for the Computer Conference must send the message: SUBSCRIBE CHEMCONF <your name> to LISTSERV@UMDD.UMD.EDU before June 1, 1993. Detailed instructions will be sent via electronic mail to registrants.

The success of any conference depends upon the quality of the papers and of the discussion. We hope YOU will help us make the summer conference a success.

DEMO OF THE NEW VERSION OF MOBY VIA ANONYMOUS FTP

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

The demonstration version of MOBY, version 1.5, may be obtained via anonymous FTP from benny.bsc.mass.edu(or 134.241.41.5). If you have access to a computer on the Internet which supports FTP (file transfer protocol), log on to the computer and use