

readily defined, e.g.

```
: SQUARE DUP * ; ...define 'square'.
: CUBE DUP SQUARE * ; ...define 'cube'.
12 CUBE . ...print 123
```

Both of these new words operate on the stack-top.

As a result of the 'word'-based structure, a Forth program is a sequence of pointers (or jumps) to brief primitive segments of machine-code. This is called 'threaded code'. Forth programs do not need to be compiled, and yet are much faster in execution than interpreted languages. Because the primitive word-segments are accessed by address, they do not need to be copied each time they are supplied to a program sequence, so Forth programs are usually very much more compact than the equivalent machine-code created by a compiler. The word-based organization lends itself very well to program development by a bottom-up approach (rather than the more widely used top-down approach of functional programming).

Forth resembles assembly language in many of its operating details and its efficiency of execution, and yet it is high-level and transferable. At first sight, Forth source-code seems dense and cryptic, but it becomes intelligible on acquaintance. Its compactness and efficiency make Forth a valuable language for numerical real-time instrument control with small computers. Forth has string and text processing capabilities and has been used as an implementation language for interpreters, compilers and text-editors.

If you consider acquiring a Forth system, pay great attention to

the systems-library of defined words, to ensure that it has the range of capabilities that you need. The Kelly and Spies text covers most of the principal Forth dialects and has an good bibliography of Forth texts and sources of software and information.

M. G. Kelly, N. Spies, *Forth: A Text and Reference*, (Prentice-Hall, 1988).

L. Brodie, *Starting Forth*, (Prentice-Hall, 1981).

HOW I USE COMPUTERS IN MY LABORATORIES

by Edward Kelly

Chemistry Department
Marian College
3200 Cold Spring Rd.
Indianapolis, IN 46222

Marian College is a small, liberal-arts college on the northwest side of Indianapolis. Despite limited resources there has been progress in developing the use of computers in my courses.

The first microcomputers purchased by the school were TRS-80, models III and IV. Eventually they were replaced by Apple and IBM computers. The Chemistry Department was offered full-time use of the TRS-80 computers. While not state-of-the-art, the TRS-80 has proved to be reliable and useful for introductory interfacing experiments. Finding a suitable interfacing circuit was my first problem. Fortunately I found one while attending a Chautauqua Short Course (Microcomputers as

Laboratory Tools, Rex Berney, University of Dayton, 1986). For about \$25 per computer I was able to interface the TRS-80 computers.

There is a strong emphasis in my labs on data collection, the analysis of that data and the interpretation of the results. The role of the computer in the lab to do the collection and assist with the analysis of data has been given high priority.

The lab manual (*Inquiries Into Chemistry*, Michael Abraham and Michael Pavelich, 2nd ed., Waveland Press, Inc., 1991), used for the first chemistry course for science majors, General Inorganic Chemistry, uses the discovery approach. Discovery experiments have the students collect data, graph the data, obtain an algebraic equation and "discover" the appropriate chemical principle. During the first semester the students do their own graphing to develop their technique; during the second semester the students use Graphical Analysis II (Vernier Software, 2920 W. 89th St., Portland, OR 97225) to learn how to use the computer to do their graphing. They always do a Least-Squares Analysis to find the best straight line through their data points; several experiments require a transformation of the data to obtain the desired straight line.

There are two types of discovery labs: guided inquiry (directions are given for the experiment, but only minimal directions are given for the analysis of the data) and open inquiry (only a statement of the problem to be investigated is given). Several of these labs have been modified to allow the use of a computer to collect and analyze the data. Additional interfacing labs have been developed and incorporated into the

lab schedule. These are described below.

The first interfacing lab covers some of the fundamental concepts of electronics and laboratory interfacing. These fundamental concepts are then used in other labs throughout the remainder of the year.

An open inquiry lab asks the student to investigate (collect the data and find the algebraic equation) the cooling curve for hot water. The data is collected using a thermistor interfaced to a TRS-80 computer. The computer controls the experiment, makes a measurement every 10 minutes, stores the data on a disk file and displays a crude graph on the screen during the experiment. Later, the students read the disk file, graph the data and find the algebraic equation.

Experiment K-1 in the lab manual investigates the kinetics of the reaction of bromocresol green and bleach. The bleach and dye are mixed and the time it takes the changing color to match a standard solution is determined. When the two colors match, the timer is stopped. This proved difficult for some students. A more effective way is to interface a Blocktronic (a photoresistor and green LED encased in two 2x4's bolted together) to a TRS-80. The internal clock of the computer is used to measure the elapsed time. The voltage output of the Blocktronic, while the color is changing, is compared to the constant voltage output of the standard. When the two voltages match, the internal clock in the computer is stopped and the elapsed time is displayed on the screen.

The oxidation of persulfate ion by iodide ion is investigated by measuring the changing absorbance with time, using the

Blocktronic (see laboratory module, LM024, Project SERAPHIM, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706). The computer collects the data and stores it on a disk file for future analysis. The initial slope of the line on the absorbance-time graph is proportional to the initial rate of the reaction. Seven reaction rates at different concentrations and temperatures are measured, enabling the student to determine the order of the reaction and the activation energy.

The molar mass of an unknown solute is determined by freezing point depression. A thermistor is interfaced to a TRS-80 computer and the cooling curves are obtained by the computer. The computer makes the measurements, stores the data and displays a crude graph on the screen. Later the student reads the disk file and graphs the data. The freezing points of the solvent and appropriate solutions are measured and eventually the molar mass of the unknown solute is determined.

A crude gas chromatograph is interfaced to a TRS-80 computer to separate a pentane-hexane mixture using a column of Tide detergent. This is a modification of procedures used by several authors (Chemtek: Small-Scale Experiments for General Chemistry, Stephen Thompson, Prentice Hall, 1990; Interfacing the High School Science Laboratory to a Computer, John Fox, Vernier Software, Portland OR, 1988). The carrier gas is natural gas. An ir phototransistor detects changes in the temperature of the flame. The changing temperature is displayed on a line printer connected to a TRS-80. Various parameters, e. g., retention times, plate thickness and the number of theoretical

plates, are measured. The computer will determine the area under the curve by numerical integration (trapezoid method). From this a crude calibration curve can be determined and the percent composition of various pentane-hexane mixtures determined.

The gas chromatograph is the last of a set of three chromatography experiments (TLC separation of washable and permanent inks, PC separation of 5 transition metal ions, and the gas chromatographic separation of a pentane/hexane mixture). The SERAPHIM computer program SEPARATIONS (AP808) is used to introduce the TLC experiment. During the first 45 minutes of a two hour lab period the class views the program projected on a large screen using a LCD in the classroom. The program reviews some basic concepts of electronegativity and polarity in order to introduce some simple ideas of chromatography. A simulation of a TLC separation of washable and permanent inks shows the considerations necessary in choosing a solvent. The students then move into the lab and apply these concepts to separate the components of some washable and permanent inks.

During the last four lab periods, the students are required to do a mini-independent research project. To introduce the students to the research process, they independently work through the SERAPHIM program LAKE STUDY (AP804 or PC3704), a simulated investigation of the cause of a fish kill. They work through an assigned worksheet outlining the details of the lake study investigation.

To assist them in selecting a research project and to acquaint them with computer literature searching and the use of key

words, the students use CHEMLAB (PC2001), a data base of labs from the Journal of Chemical Education.

In the Physical Chemistry Laboratory, students work with computers in a variety of ways. This course is taken in their junior/senior year. By that time they have had a programming course, either BASIC or Pascal. They are asked to write several computer programs during this course.

The first computer assignment is to write a program to find the root of an equation (volume in van der Waals cubic equation) by four different algorithms: (1) successive approximations, (2) bisection, (3) tangent, and (4) Newton. They are given two modules: ITERATION AND COMPUTER PROBLEM SOLVING, and ALGORITHMS FOR FINDING ZEROS OF FUNCTIONS (#478 and #264, respectively; COMAP, Inc., 60 Lowell St., Arlington, MA 02174), which describe these methods. They are asked to compare the methods for speed of convergence, accuracy, etc.

The second computer assignment requires the student to find the root of an equation (the solubility of an insoluble salt whose anion interacts with the solvent). They must write the six equations involving the various equilibria (solubility product, two acid dissociation equations, dissociation of water, mass balance and charge balance). (See, for example, Fundamentals of Analytical Chemistry, Douglas Skoog, Donald West and James Holler, Saunders, 6th ed., 1992, chapter 8.) The six simultaneous nonlinear equations must be reduced to one very nonlinear equation, whose root is determined by one of the methods mentioned in the previous paragraph.

The next computer assignment

involves numerical integration. The students are given Cp-T data and a module, ELEMENTARY TECHNIQUES OF NUMERICAL INTEGRATION AND THEIR COMPUTER IMPLEMENTATION (#379, COMAP), and told to determine the entropy. The module describes three methods of numerical integration (left-rectangle method, trapezoid rule and Simpson's rule); the students write a program using the three methods and compare the results.

The students are asked to find experimentally the K_{sp} of $\text{Cu}(\text{IO}_3)_2$ by potentiometric titration. An ADALAB card interfaces the electrodes to an Apple computer. The computer stores the data, displays a graph of emf versus volume of titrant (making it easier to follow the titration and select an appropriate volume of titrant for the next addition); when the titration is over, the computer prints out the emf-volume data, including the average first and second derivatives of emf versus volume. The endpoint can be determined very accurately from the derivatives.

The students use a computer program that demonstrates the Monte Carlo simulation of a variety of chemical reactions. A module, MONTE CARLO: THE USE OF RANDOM NUMBERS TO SIMULATE EXPERIMENTS (#269, COMAP), describes the Monte Carlo method. The Monte Carlo method is applied to five chemical reactions; some simple first and second order reactions so that the Monte Carlo results can be compared to the results from the integration of the appropriate rate equation. Then more complicated reactions, that are not easily solved analytically, are "solved" by the Monte Carlo method to demonstrate its power.

The data from a kinetics experi-

ment (the oxidation of $\text{S}_2\text{O}_8^{2-}$ by I^-) is analyzed, using two statistical techniques: analysis of variance and factorial design, to investigate the interaction of temperature and catalyst concentration on the reaction rate. Spreadsheets are a very convenient way of obtaining the required sums, sum of squares, squares of sums, etc. needed in this statistical analysis.

To illustrate the power of the computer in doing quantum chemical calculations, the students are asked to find the minimum energy of the He atom by a self-consistent-field linear-combination-of-atomic-orbitals molecular-orbital (SCF-LCAO-MO) calculation using the trial wave function $C_1e^{-\zeta_1 r} + C_2e^{-\zeta_2 r}$. One needs to guess the values of ζ_1 and ζ_2 , then find the C_i 's and the energy by iteration. The students are given the computer program that optimizes the C_i 's and energy for a given set of ζ 's. The students spend one lab period trying to determine by whatever method they choose the best set of ζ 's, i. e., those that give the lowest energy. The following week they are given another computer program which uses a simplex optimization algorithm to find the best set of ζ 's. They are then asked to compare the methods.

In Analytical Chemistry Laboratory the computer is used for record keeping and calculations. A potentiometric titration of iron is done by interfacing the electrodes to an Apple computer by an ADALAB card. The computer stores the data, displays a graph of emf versus volume of titrant. At the conclusion of the titration, the emf-volume data is printed out, including the average first and second derivatives of emf and volume; these derivatives enable the students to more accurately determine the endpoint of

the titration.

Copies of the laboratories described here are available from the author upon request.

COMPUTER CONFERENCING AND THE COMPUTER CONFERENCE ON APPLICATIONS OF TECHNOLOGY IN TEACHING CHEMISTRY

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 (TOH@UMD2.UMD.EDU)

INTRODUCTION

An announcement of the Computer Conference on Applications of Technology in Teaching Chemistry appears elsewhere in this issue. This is the first such conference sponsored by the Division of Chemical Education's Committee on Computers in Chemical Education.

Computer conferencing has been used in education, business, industry, government and the military. Many of the applications in education are directed towards course work and degree programs. A few references are presented at the end of this article. Some of these references contain extensive bibliographies. SELECTION OF CONFERENCING SOFTWARE

The authors are interested in conferencing software which is available at little or no cost and is accessible to a wide variety of chemistry educators. It was decided to use LISTSERV since it can serve those having BITNET or INTERNET addresses.

LISTSERV is used by the Chemistry Education Discussion

List (CHEMED-L). Many chemists are already familiar with some of the features of LISTSERV. In the configuration we are using anyone can establish a CHEMCONF LISTSERV account and can remove himself from CHEMCONF. When mail is sent to CHEMCONF it is automatically distributed to all those on CHEMCONF. Each piece of mail is indexed and filed in a "notebook." Users can obtain the index (or part of the index). A file can be retrieved from the "notebook" and printed. Also, it is possible to obtain the names and electronic mail addresses of all those who are signed on to the LISTSERV account. Under favorable conditions messages are distributed within a few minutes, but in some cases longer delays may be observed. Thus, it is not possible to carry on a "real-time" (synchronous) conversation in the usual sense. However, this may have the advantage of encouraging more thoughtful replies.

LISTSERV is almost strictly a text oriented facility. Graphics mostly in the form of slides and transparencies are important to most presentations at meetings. The authors have identified the software which will convert a graphic image to an ASCII character file and additional software which will produce the original graphic image from the ASCII file. Much of this software is either in the public domain or available at a small cost. We have developed simple instructions to assist authors and participants in using the software. Graphics, chemical structures, spreadsheets, executable binaries, HyperCard stacks and digitized photographs can be handled. In addition to these instructions, individual help will be available through the conference manager (Tom O'Haver).

FORMAT OF THE MEETING

The meeting will be divided into two sessions. Each session

will consist of five papers and will extend over a period of three weeks. On the first day (a Monday) all five papers will be distributed to all participants. Each paper will consist of an ASCII text file which may contain tables. Each graphic will be transmitted as a separate ASCII file which will have to be converted by each participant. Participants will have the remainder of the first week to read the papers. Authors are encouraged to stimulate discussion by including questions for the participants in their papers. Participants will have an opportunity to send short (less than 100 word questions) to the author or other participants on a designated day during the first week.

The second and third weeks will be devoted to asynchronous discussion and questions. Two days will be devoted to discussion of each paper. This format has some distinct advantages over a conventional on-site conference.

- Each participant will have a week or more to read the paper and prepare any comments, suggestions or detailed questions. The participant will be able to research and carefully word his comments and questions. Relevant references can be located and cited to reinforce a point of view.
- Authors will have time to consider responses to questions.
- Since discussion will occur over two days, there will be time for an extended dialog and considerable discussion.
- All papers and discussion will be saved in files until the end of the conference. Participants and authors will be able to access these files at any time.
- Authors planning to submit their papers for publication subsequent to the conference may receive de-