Tables II, III, and IV suggest some uses before, during, and after the lab.

Graphing results from kinetic experiments, titrations, and apparatus and instrument calibration during the lab will suggest how effective the work has been or whether it should be repeated. Searching for spectra to compare to observed spectra would give feedback as to how successful a synthesis had been. Some students might keep electronic notebooks.

Computer stored or generated spectra and molecular modeling programs could be used for preparatory assignments or dry labs. We have had students use qualitative organic analysis simulation to increase the efficiency and effectiveness of unknowns in the lab.

Students are asked to come to the Organic lab having done prior preparation. This preparation usually includes finding the chemical and physical properties of the substances to be used or prepared. Now we need to add to that, information on toxicity and methods of disposal. Computer searchable data bases could facilitate this process.

Participants at the conference in August were asked to fill out a related questionnaire. A few did. The questions were:

1. What software programs do you use in conjunction with teaching the Organic lab?
2. How would you like to use the computer in this activity?
3. Do or should your students have access to computers "in" the Organic lab as they do to IR and GC?
4. How would you like your Organic lab students to use computers?
5. What stands in the way of more use of computers in the Organic lab?

Responses for question 1 included different spectral programs (mentioned by all but one responder and one of these mentioned the Sadtler Library Search program), Beaker, word processing, and drawing programs. One respondent said they had a qual organic search program for compound identification containing data for 6000 compounds stored on their IBM mainframe.

Suggestions for question 2 included input data and check calculations or receive suggestions (i.e. error, possible compounds), analysis of gas chromatographic data, simulations, modeling, lab notebook, and to identify spectral unknowns before doing qual. The responder with the ID file said their students get a list of possible compounds. That sounds interesting.

Answers in response to question 3 range from no response through yes (several) to one lab which is connected by cable to mainframe with input from the lab.

Question 4 drew responses expanded from #2. They include: Preview lab set-up, compare and average class results (Good for discovery labs!), grade their own preparations with IR and NMR as resources, write lab reports, spectral searches and simulators, and using the library that comes with FT-IR.

In response to number 5, almost all said space and/or money. One threw in the administration. No one mentioned concern for damage to the computers. One honest responder spoke for all of us—"my inertia."

Don't let your inertia get in the way. Write today if these topics are of interest to you. If people are interested, I would be willing to act as a clearinghouse and seek to air your ideas and concerns (quality of software, software needed, ways to use them, successes, etc.) in print.

Windows and Networks: Lowering the Activation Energy for a Chemistry Department Microcomputer Facility.

T. C. O'Haver, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742 (to2@umail.umd.edu)

Abstract

A synergistic combination of a window-oriented user environment and high-speed local and wide area networking is the technological basis for a successful faculty-student computer workstation room in a university chemistry department. This paper describes the equipment, software, organization, operation, and application of the facility.

A. Introduction

How can a university chemistry department make the best use of modern personal computer technology to help support its teaching, research, and service mission? There is no question that computers can perform many useful tasks for the scholar and researcher, but how can we insure that the technology will be utilized in an effective way and will actually contribute to productivity? It is essential that the real benefits to the users be weighed against the increased burden of complexity that unavoidably accompanies any high technology development. Ours is a large research-oriented department of chemistry and biochemistry with 45 full-time faculty members, 200 graduate students, and 400 chemistry and biochemistry undergraduate majors. Students and faculty in our department typically have no formal computer training, are not really interested in the computer per se, and are often too busy to read manuals. Computers are not part of the mainstream of our discipline, so time spent learning about the computer is often considered time wasted. The ideal system for our purposes would be powerful enough to meet most needs but relatively intuitive to operate, so users can bootstrap themselves into literacy without wasting too much time. We clearly needed to capitalize on the benefits of the personal computer revolution: namely, the wide range of user-oriented application software. It is important that the facility exhibit a low intimidation factor so as to reduce the energy barrier to computer use. Additionally, in our situation there is no possibility of a full-time computer administrator, so the computer facility would have to be relatively easy to maintain with existing personnel. Although many of our faculty had already purchased personal computers for their offices and labs, we felt that a public computer facility could serve most of the needs of graduate and undergraduate students and would provide a common area for sharing expensive peripherals such as high-quality printers, plotters, and scanners.

B. Application goals

One area of computer application that is useful for both students and faculty is scientific communication: writing papers, reports, and proposals, preparing posters and slides for presentations, and developing computer-based lecture demonstrations. Scientific papers often involve mathematical equations that are difficult to type with a typewriter or ordinary word processor and usually include line drawings and plots (graphs) of data or calculations. Chemistry writing tends to be especially complex typographically, with lots of Greek letters, math characters, subscripts and superscripts, italics and boldface, and drawings of chemical structures that are embedded into the text as an integral part of the document. These requirements suggest that a high degree of graphics capability will be desirable. Popular text editors designed for programmers and word processors designed for the business office do not meet all these requirements. The recent trend toward graphics-oriented microcomputer environments and "what you see is what you get" operation is very beneficial in this respect. We felt that this was even more important than raw operational speed and the "keep-your-hands-on-the-keyboard" ethic of products designed for the professional typist. We could meet this software requirement with either a single large technical document preparation application or with a set of separate applications that can work together to produce the finished product.

In addition to scientific document preparation, we expected to be able to use our computers to perform some of the more traditional scientific computer applications, including data reduction and "number crunching"; simulation (e.g. of molecular spectra); molecular modeling (3-D model building, energy minimization); curve fitting; statistics and exploratory data analysis; symbolic math and equation solving; digital signal processing; DNA analysis and plasmid map drawing, and kinetic analysis. For the computer programmers among us, we would need conventional programming languages as well as authoring systems for developing custom applications and courseware. Although conventional computer aided instruction (CAI) was not a high priority, we also wanted to be able to use the facility for instructional purposes where particularly effective software is available. Clearly, with such a wide range of potential applications, consistency of operation between all software packages would be a key factor. This suggests that an environment based on a modern graphic user interface (GUI) might be most appropriate, such as MS-Windows, the Macintosh, or one of the developing Unix-based GUIs (1-3).

C. Equipment

The deployment of computer workstation resources on our campus is based on workstation clusters located in various departments, libraries, and dormitories throughout the campus. Most of these are public, walk-in facilities that serve all students and faculty. Departmental personnel operate those facilities located in academic departments and offer a discipline-oriented mix of software and peripherals. A typical cluster contains 10-50 workstations and one or more laser printers. The current equipment the chemistry departmental workstation room consists of 23 Macintosh II computers (4). Each machine has a 32-bit CPU and data bus, floating-point math chip, dual 800K floppies, an Ethernet card, and 5 MBytes of random access memory (RAM). These machines are networked with a single file server and print spooler with 200 MBytes of disk storage, one LaserWriter IINT Postscript laser printer, a flat-bed scanner, and a CD-ROM drive. One of the stations is equipped with a 19" monochrome monitor that can display two entire 8" x 10" pages side-by-side, which is useful for those working with large drawings, molecular models, spreadsheets, or complex page layouts. (All the application software works with this monitor without special drivers, a consequence of the windowing environment). Another station is equipped with a Textronix Cache system, a co-processor board designed for high-performance molecular modeling. There are also facilities for reading and writing MS-DOS (IBM-PC) format floppy disks (3.5" 720K and 1.44 Mb, and 5.25" 360 K formats). The particular model of the Mac II we have used is now no longer sold; the closest current model is the Mac IIsi or the Mac II ci, which are both less expensive and about a factor of two faster than our model.

D. Application distribution
One of the important choices to be made when designing a microcomputer cluster for general access is the method of distributing commercial application software to users. There are three distinct possibilities:

1. Set up a floppy disk lending library. Users would check out floppies from a central desk and return then when finished. This requires no special equipment and would meet the licensing requirements of any commercial software, that is, that the number of simultaneous users not exceed the number of copies purchased. However, we considered this to be an unacceptable solution because there is no practical way to guarantee that unethical or ignorant users will not copy the commercial software and because of the likelihood of maintenance problems cause by accidental deletion of needed files and the introduction of junk files and viruses. Moreover, much of the best software is simply too big to run from a floppy disk.

2. Provide each workstation with its own hard disk and install the software according to the number of purchased copies of each application. Each station would have to be labeled with the particular mix of software installed on its hard disk. This would share all the difficulties of the previous approach except the last. Experience in other public microcomputer facilities of this type had showed that the maintenance of multiple hard disks is a substantial problem.

3. Connect the workstations together in a local area network (LAN) and put all the applications on a file server that can distribute them electronically. Each workstation would not require its own hard disk, because they can be booted from a floppy disk or over the network. The main advantage to this approach is that all access to the application software is strictly through the network and the fileserver, so that it is in principle possible to copy-protect the commercial software, to lock and write-protect the server against modification by the user, and to control the number of simultaneous users according to the number of copies purchased, provided that the file server software offers those capabilities. Every software application would then be available at every workstation, limited only by the requirement that the total number of copies in use at a given time not exceed the license or number of copies purchased. (The license requirements of some software, however, explicitly forbid network operation). An additional advantage is that the cost of a single large file server hard disk is less per byte than smaller disks. A disadvantage is that it requires some additional hardware and software for a file server, as well as network connections and client software for each workstation. Moreover, it depends on well-behaved application software that works well in a shared environment. This is the approach used in our facility.

E. Networking
Early tests by our computer science center showed that the Mac's built-in 230 Kbps LocalTalk network port did not provide the required level of performance for a network of our size. As a result, the decision was made to standardize on 10 Mbps Ethernet interfaces for each individual workstation. Ethernet is the departmental networking standard throughout the University and Ethernet wiring (based on thin cable) is already in place in most offices in our department. Each workstation has an add-in Ethernet card and connects directly to the departmental Ethernet. Local network services operate on AppleTalk phase 1 protocols, using the AppleShare 2.0 file sharing software, the LaserShare print server and spooler, and the Internet Router, all of which run concurrently on one dedicated Mac II acting as the "Server". This software implements transparent "remote device mounting", in which the file server's hard disk and the laser printer seems to be connected directly to each workstation, so that disk operations and printing are done in the same way as for a stand-alone computer. A utility called KeyServer provides the software checkout counting and user notification required for proper application distribution and also keeps a

record of how often and when each software program is used. The print spooling software makes it practical for one LaserWriter to be shared by the 23 workstations. The router bridges the Ethernet to the LaserWriter, which connects to the fileserver via the usual LocalTalk connection. Since it sees only printer traffic and not file server traffic, the LocalTalk connection is adequate in this case. No additional hardware bridges or routers are necessary. In addition to the 23 Mac II's in the public workstation room, computers of all types in individual faculty or staff offices can be connected to the Ethernet with the appropriate network adapters in order to have access to TCP-IP services or the laser printer.

Note that we use file server primarily for application distribution rather than document sharing which is the standard model for office networks. We expect walk-in users to save their document on their own disks (which they provide) and to take them with them when they leave. Each workstation has two built-in floppy drives, one for the boot disk and one for user files. Each station also have a SCSI (Small Computer System Interface) port, which can be used to attach an external hard disk drive. Users who are working on very large files sometimes bring their work in on a small portable hard disk which they connect to their station while they are working. We do not provide long-term private user file storage on the file server. However, we have created a public subdirectory (folder) called the Temporary Storage Folder that users do have write privileges to. This is useful for temporary storage while working on large documents, facilitates the use of applications brought in by the users on floppy disks, and can be used as a convenient means of informal document sharing between users throughout the building.

F. Wide area access

In addition to the AppleTalk-based network services described above, we use TCP-IP protocols to provide access to the Chemistry Department VAXs, the campus electronic mail system, the library card catalog, the campus electronic bulletin board, any of the campus host computers, and national networks such as Internet, Bitnet, NSFnet, SURAnet, etc. Each station on the network is assigned a unique IP number for TCP-IP services. Anyone on campus can obtain a personal account on one of several Unix-based host systems that support mail servers. We use the MacTCP drivers and a public-domain terminal program (NCSA Telnet) to access the various departmental and campus computers. An FTP front end program provides a convenient point-and-click interface for downloading files from remote hosts on the Internet.

The connection between the departmental Ethernet and the campus broadband network is performed by a dedicated gateway machine that passes TCP-IP traffic but not AppleTalk traffic. Access to our departmental file server and printer is therefore restricted to workstations that are physically connected to the departmental network; this is desirable considering that it is the department itself that purchases the application software and the paper and toner for the laser printer. For similar reasons we currently do not have the ability to dial in to the file server or print spooler from outside the university via telephone.

G. Application Software

Currently, the departmental file server provides the following application software: Scientific word processing with spelling checking; math equation formatting; organic structure drawing; molecular modeling (with 3-D graphics, MM2 energy minimization, and molecular dynamics trajectories); general-purpose paint and draw programs; graphic scanning; optical character recognition; DNA analysis; plasmid map drawing; data plotting and least-squares fitting; spreadsheet with graphics and macros; statistics and exploratory data analysis; non-procedural equation solver; a vector/matrix processor with graphics; digital signal processing; electronic system simulation; computer languages and authoring systems for developing custom applications and courseware; a student expert system for organic chemistry ; first- and second-order proton NMR simulator; a mass spectroscopy fragment identifier; educational courseware for organic chemistry and organic spectroscopy (proton and carbon NMR, MS, IR); Hückel MO calculator. Each of these packages has been purchased in a quantity dependent on its anticipated level of use: in some cases enough copies for the entire room, and in other cases a single copy (in which case only one user at a time is allowed by the file server). In addition to the commercial software, we have collected several MBytes of utilities and science- related public domain software that users can copy, as well as a collection of chemistry "clip-art" organized in a Hypercard stack, for use in illustrating reports and lab manuals, etc. Some additional applications were suggested by the availability of the technology rather than a perceived prior need: in particular, graphic and text scanning, using the scanner to capture, reduce, clean up, and annotate large chart recordings, gel electrophoresis plates, etc, for insertion into a report or thesis; optical character recognition for converting printed text into editable word processor files, and conversion of scanned graphs and plots into numeric data tables.

H. Memory and disk space requirements

In additional to the usual random access memory (RAM) requirements of applications running on a stand-alone personal computer, the individual workstations must additionally have enough RAM for the Ethernet driver, the AppleShare client software, the TCP-IP driver, and an automatic virus checker. As delivered, the computers had only 1 MByte of RAM, but we gradually expanded them to 5 MBytes, which allows easier operation with very large data files. One MByte of that RAM is allocated to a virtual disk (RAM-disk) on which the boot disk files are stored. This makes some operations much faster, and it frees up one disk drive, because the boot disk ejects automatically after its files have been transferred to the virtual disk in RAM.

I. Performance issues

So far all the software that we have tested works well from the server. Several simultaneous users can use one copy of a program on the server (subject to the license requirement). Most applications work from a write-protected volume or folder (that is, one for which the user does not have "make changes" privileges). Tests have shown that launching programs from the file server is nearly as fast as having a hard disk on each station. Network slowdown when the lab is very busy is noticeable but not objectionable. Overall reliability is good, but there are occasional temporary lapses of file service. Computationally, the Mac II is roughly as fast as an old MicroVAX, based on standard math benchmarks.

J. Maintenance

All such facilities require a certain amount of routine maintenance. The administrator can install new application software and upgrades and set up access privileges to volumes and folders from any workstation on the network, simply by logging on to the file server with a password. However, the administrator can copy protect the commercial software only on the file server itself. We do not give users write privileges to the file server, except for the Temporary Storage Folder, which the administrator must periodically clean out. The boot disks require periodic checking for viruses and stray files left behind by users. Viruses have been a problem. They can be spread from a user's disk to the boot disk and thence to another user's disk. An automatic virus checking *init* on each boot disk is a necessity. We update these regularly to respond to new virus strains. The boot disks get rather heavy use and tend to become corrupted or wear out eventually; a supply of backups is always on hand. Because of the problem of boot-disk maintenance, we are currently in the process of installing a modification that allows each station to boot directly over the network, without using any local storage disks. This modification will eliminate the boot disk maintenance problem and will make it much easier to install global changes in boot configuration to the entire lab, such as changes in system version or font selection.

Hardware and software upgrades and expansions have caused no problems. The author accomplished the installation of additional memory, an additional server hard disk, a CD-ROM drive, a scanner, and a large screen monitor with no difficulty.

K. Operation

The workstation room is a public facility that is open to all students, faculty and staff on a walk-in basis. No charge or authorization is required to use this facility. Undergraduate students hired as attendants are present during normal hours of operation. We leave the server on 24 hours a day, seven days a week, so that networked users outside the room can have access to the server and print spooler at all times. We keep manuals for all the software nearby. One wall of the room is equipped with a large corkboard which we have covered with screen dumps and sample print-outs of software doing chemistry-related work. We have prepared a substantial number of handouts that explain such topics as basic workstation operation, how to type special characters, transferring graphics from one application into another, operating the scanner, plotting data, typing equations, creating a spreadsheet or equation solver model, file transfer, etc. Copies are available in the room and are archived on the FileServer so users can view and print them out from any workstation. For the novice and first-time user, we have found that the "Guided Tour" disks that come with the computers are very useful. The Chemistry Department offers no user training classes. The Computer Science Center does offer free peer training classes for students, as well as more formal classes and workshops in a variety of topics. Most users learn by watching other users and by experimenting.

L. Curriculum integration
We base our strategy for integration of computer use into the chemistry curriculum primarily on the use of commercial application software to support instructor-developed exercises. We emphasize the use of the computer as a student-directed tool rather than for lesson presentation, sequencing, and grading (5). For example, in our undergraduate organic chemistry classes, students perform a kinetics experiment in the laboratory, then bring their data up to the workstation room to key it into a general-purpose data plotting program to transform and plot the data, do a least-squares curve fit, and compute the activation energy of the reaction. These students are also exploring organic nomenclature and reactivity using Beaker 2.0, a type of expert system for organic chemistry students. The graduate organic class has been using molecular modeling and MM2 energy minimization to investigate structural concepts (6). Students in the environmental chemistry class use a spreadsheet to compute and plot elemental enrichment factors for atmospheric particulates using instructor-prepared data sets (7) and to investigate the influence of atmospheric chemistry on the pH of rain, using the Charson-Vong equilibrium model implemented in a non-procedural equation solver. An elective "electronics for chemists" class uses an electronic system simulation package to investigate signal-to-noise ratio enhancement systems, such as tuned filters, AC detection systems, and lock-in amplifiers (7). Students in a laboratory computer interfacing course investigate digital signal processing using a locally-developed program called SPECTRUM (8).

Most conventional CAI chemistry education software, such as the materials from SERAPHIM and JCE software, runs on Apple II or IBM-PC platforms. Third-party emulation software is available that allows these programs to run on the Mac II. We evaluated Insignia's SoftPC DOS emulator and found that it did indeed run all the MS-DOS programs we tried; moreover, it allowed convenient copy and paste of text and graphic between MS-DOS and Macintosh programs. Its screen update speed is somewhat poorer than one expects on a modern PS/2-class machine, but this is nevertheless a very inexpensive way to provide basic PC software compatibility.

M. Conclusion
The workstation room described here has been in continuous use since 1989 and has become a very popular facility. It offers a reasonable compromise between human factors (ease of learning and ease of use), computational performance, and the scope of available software applications. There is also ample opportunity for future hardware expansion: each workstation has 4 unused expansion slots for add-in cards and there is room on the motherboards for 8 MBytes of RAM using conventional 1 Mbit memory. As many as five more hard disks could be attached to the server's SCSI port. Future developments in hardware and software will certainly offer greater computational performance, but our hope is that the human factors will receive continued and even increased attention. Even the most "user friendly" computer can still sometimes be very frustrating, especially for the novice user and occasionally even for the more experienced user.

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