University of Kansas, Lawrence, KS Robert Megargle - Cleveland State University, Cleveland, OH Thomas C. O'Haver - University of Maryland, College Park, MD Brian Pankuch - Union County College, Cranford, NJ Harry E. Pence - SUNY College, Oneonta, NY Kenneth Ratzlaff - University of Kansas, Lawrence, KS Donald Rosenthal - Clarkson University, Potsdam, NY Barry Rowe - Champaign Centennial High School, Champaign, IL Gwen Sibert - Roanoke Valley Governor's School, Roanoke, VA Allan L. Smith - Drexel University, Philadelphia, PA Stanley Smith - University of Illinois, Urbana, IL Carl H. Snyder - University of Miami, Coral Gables, FL William J. Sondgerath - Harrison High School, West Lafayette, IN Theresa J. Zielinski - Niagara University, NY.

CONCLUSION: To be successful the CCCE must meet the needs of chemical educators. We rely on your contribution to and participation in our activities.

EDITOR

An interesting use of advanced graphics.

by Brian Pankuch,
Department of Chemistry, Union County College, Cranford, NJ 07016
pankuch@hawk.ucc.edu

Princeton:

I arrived at the Art History class just at the start of the lecture. Kirk sat me down in front of the Silicon Graphics computer, toward the back of the room. The lighting was subdued, which made the 20" color screen quite bright. The main reason for the dark room was not for my screen but for the 20 foot projection screen at the front of the class. The projector itself was mounted out of the way from the ceiling.

He showed me some of the basics then hurried to the front to take his position with the powerful Silicon Graphics computer controlling the projection screen. Alice, a professor of Art History, explained we were to explore a database containing high quality reproductions of paintings, frescos, the buildings holding the art, artists who made it, people who commisioned it, or posed for it, etc.. She explained the overall tour and Kirk simultaneously showed demonstrations, on the projection screen, of methods we would use. Peter, the programmer of the database, moved around answering questions and making suggestions. My position toward the back of the room had the disadvantage of my not being able to read fine print on the projection screen, but had the advantage of being able to see what others were pursuing on their screens. Their were 7 students and 4 professors visiting from other universities and other departments at Princeton.

Some followed step by step with students generously helping visiting faculty find the correct material. Others flew into the system opening a wide variety of examples on their screens. We started by opening a few reproductions. The machines seemed quite slow to me, Peter confided to me that they were severely under strength for RAM- a mere 16 Meg. He feels they need at least 32 Meg each locally while being connected to a 12 processor server.

We proceeded to open architectural drawings of the building housing some frescoes. Alice confides this is the area that first caused her to request Kirk to help out with some computer simulation. Kirk uses his system to zoom into the building- very realistic on the large screen. It is a 40 ft high ceiling , a long building with frescoes on both long walls, stained glass windows at the end to provide some of the light.

Kirk changes the perspective and we turn to view the frescoes on the right wall. He pans up to the left corner sweeps the whole wall and Alice discovers some of the frescoes are in the wrong order-Kirk moves the frescoes, Alice discovers some more errors and Kirk expertly moves the frescoes again to the correct order. The frescoes are read starting at upper left to the right, then the next row below are read from left to right, then back at the left side we read the next row to the right. I didn't know that- but it makes sense, the building is long, it is easier to read this way. (Some ancient writings apparently were also written this way) . Alice had tried to do this with single photographs but felt it was not very clear.

Kirk adds that he can change the lighting for us - his system has the ability to make a light and realistically place and change resulting shadows, as we move. He shows us the affect as he speaks. The changes are quite effective, I want to try it on my machine. Peter laughs, it seems Kirk's machine has 128 Meg, compared to my poor 16 Meg. Kirk continues to add light sources and change our viewpoint. He reminds students not try the changes he is doing because they could affect the whole database. Maybe art students are different, but the computer science and engineering students I've worked with at Princeton would find this an irresistible challenge. I will have to check back and see if mysterious lights are appearing from unlikely places.

My system does allow me to continue doubling the size of the picture, and to scroll through at great magnification that allows me to see details that Alice is putting into context. Peter stays close to me because I keep exploring in all directions and crashing his neat interface. I find many relations I try to

explore have no connection. Is this due to my lack of knowledge in the area or am I just pushing the system too far?

Alice and Kirk get into a discussion with some of us about how decisions were made to use the data in the relational database. It turns out that 700 or so pieces were put in, it could easily be 30-40,000. One reason at least why some connections were null.

The interactions with the system are interesting, the mouse we use has 3 buttons instead of the usual one. This allows some interesting abilities my Mac doesn't have, but it also leads to some problems if you get too many things going at the same time. Practice and learning more about the interface will help. Now its been 3 hours since the class started, this is the 3rd different system I've looked at today and I've got one more to go. Peter invites me back to play some more and discuss the interface. Sometimes I think programmers have a sadistic streak.

The students are left with the assignment to answer a number of questions by exporing the database on their own. Kirk shows where to leave messages if they come across possible errors such as the frescoes being out of order. It is interesting and challenging being only a few days ahead of the class.

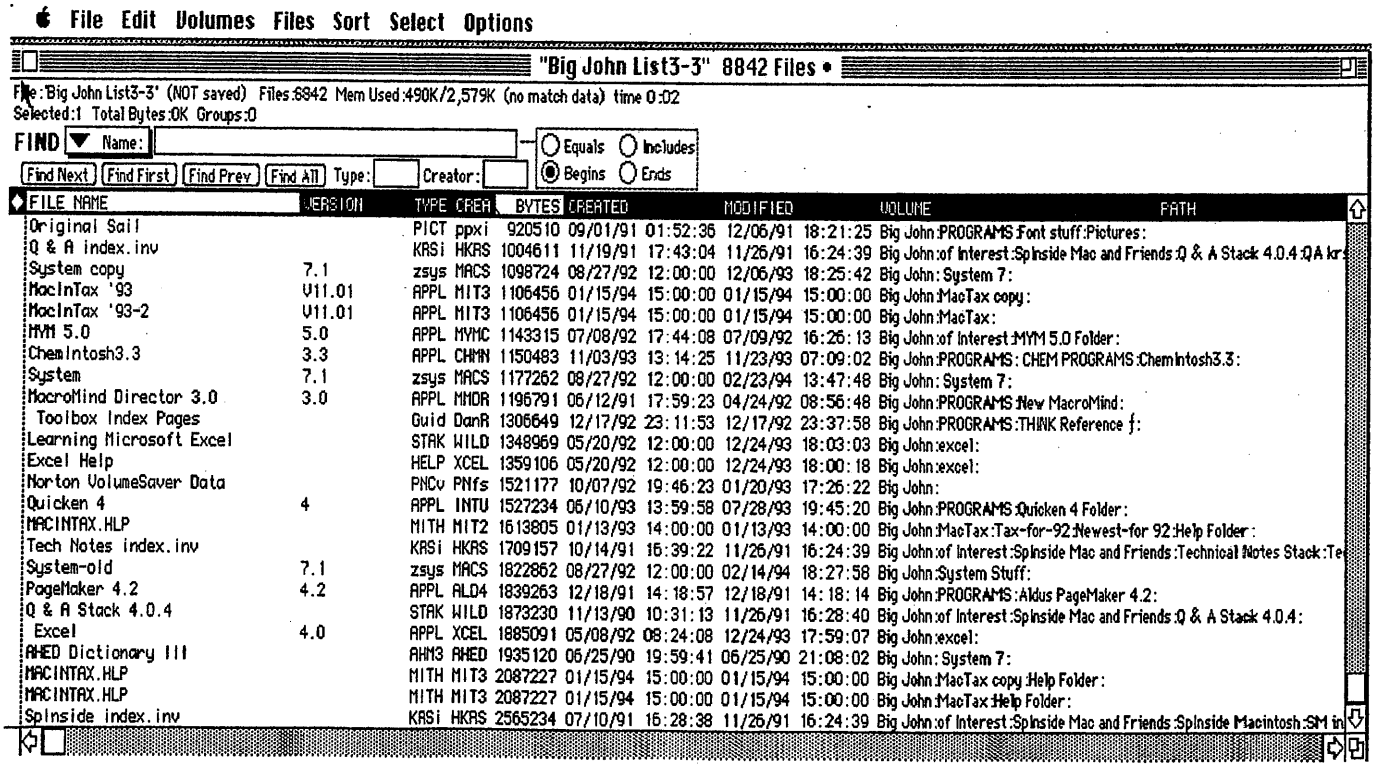
Why Art Histroy-because they are actually doing visualization with an undergraduate class. Imagine the building as a large molecule, we can enlarge our way to individual atoms, select an atom, a bond or a whole section of the molecule, and search an attached database for 'connections.' I have used databases about the periodic table - not particularly visual, but very interesting.

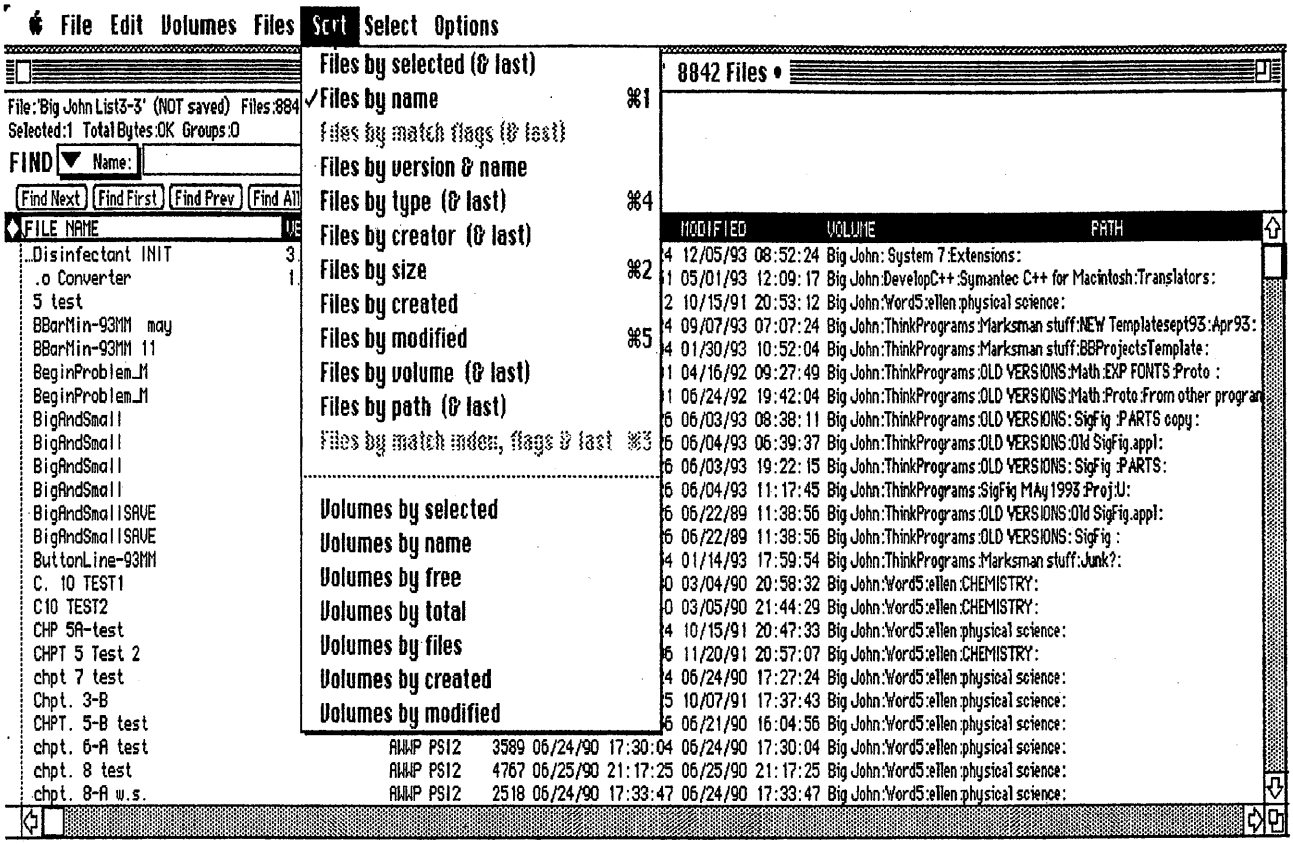
USEFUL UTILITY:

FileList+ 1.0b21 is a utility I came across more or less the same time I realized that I had over10,000 files on my hard disk. FileList puts all your files with a great deal of information into an easy to use database. You can then easily see duplicates, strange files you were going to look at but never got to because they are now buried at the 8th level of the file system. You can rapidly set up search criteria and find special files. I was able to get rid of over 1200 files , about 70 Meg, in less than an hour.
Sorting by name can pick up duplicates, by size the files that can free up the most space. You can sort by several criteria at the same time.

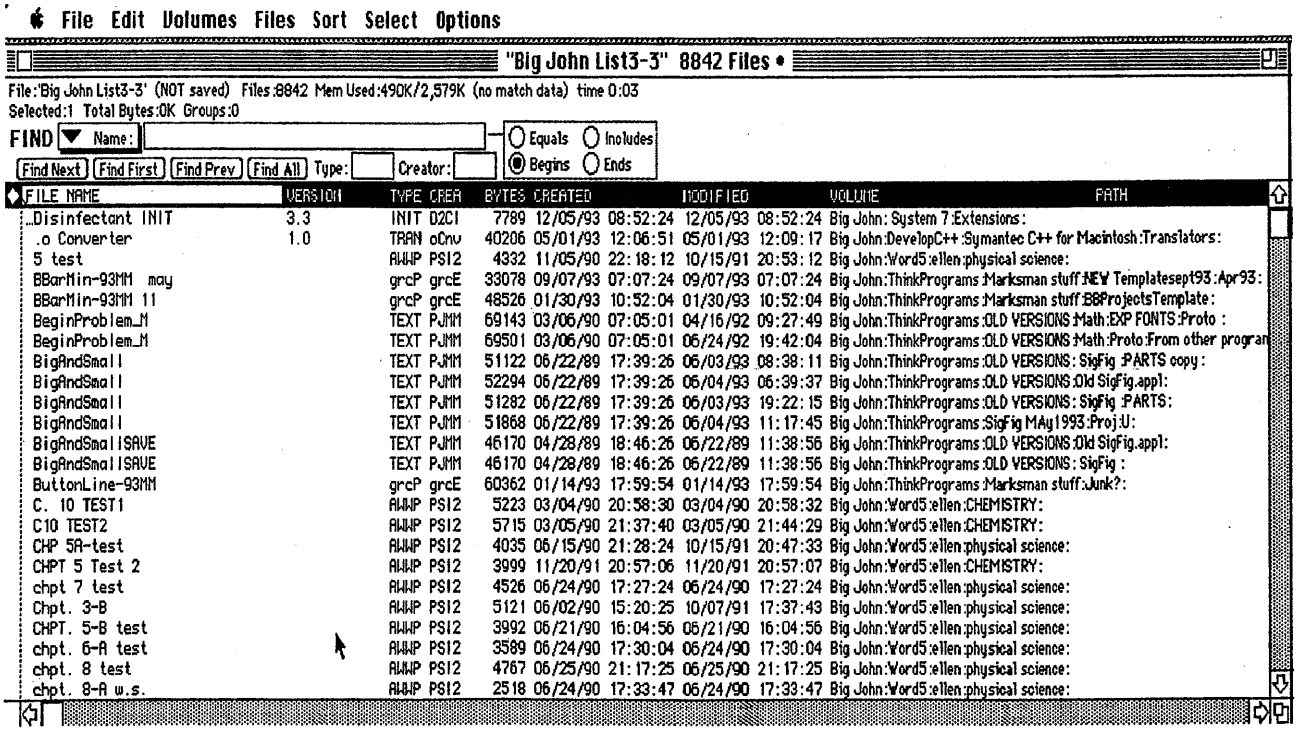
The authors ordering information follows: "If you want me to send you the latest version of FileList+, send me an 800K or 400K floppy with an stamped mailer and I will be glad to send it to you. Please let me know if you want the last release or want to wait for the next one (if one is coming). If you donate $5 or more, I'll spring for the floppy, mailer, and postage and send you the latest, providing you request it." Mail to: Bill Patterson 805 Division St. Greenville, TX 75401

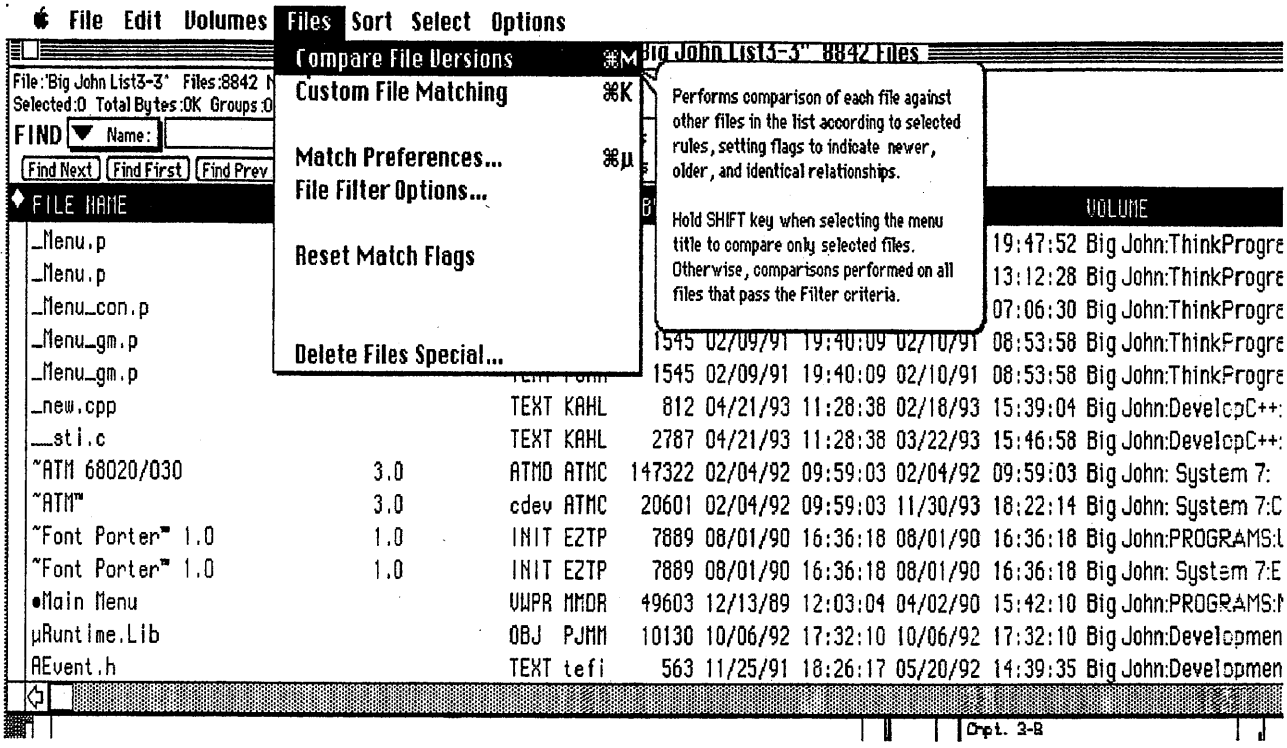
Below are some screen shots of the utility in use.





This shows some of the many ways in which you may sort your files. Below are the files resorted by name taking only





The utility includes balloon help shown above explaining one of the listings below the menu heading files.

NOTE: Henry R. Derr, Laramie County Community College, Cheyenne, WY 82007 HDERR@eagles.lcc.whecn..EDU, WOULD APPRECIATE EVERYONE WHO HAS EMAIL TO SEND YOUR EMAIL ADDRESS TO HIM. THANKS

MOLECULAR DYNAMICS SIMULATION ON A MICROCOMPUTER

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

Molecular dynamics simulations are important tools for under standing the behavior of large biomolecules. I have adapted a molecular dynamics simulation of the denaturing of a protein alpha helix (1) for use in a senior biochemistry course for chemistry and biology majors. The exercise consists of five parts:

1. Construction of a polyalanine alpha helix by template forcing.
2. Energy minimization of the alpha helix.
3. molecular dynamics simulation of denaturation.
4. examination of hydrogen bond lengths before, during and after the simulation.
5. viewing a "movie" of the denaturation.

A polymer of 15 alanine units was constructed by duplicating and connecting a minimized alanine structure found in a library of structures. Then a 15 amino acid alpha helix was "clipped" from cytochrome C for use as a template. By assigning constraints between corresponding atoms in the two polymers, the polyalanine polymer was forced to assume the conformation of the template alpha helix.

Then the template was removed, and an energy minimization was done on the polyalanine alpha helix. This adjusted the structure to a local energy minima for the actual methyl side chains. The use of an idealized alpha helix, with identical non-polar side chains, focuses the exercise on what happens to the hydrogen bonds between amides as the helix starts to denature.

Then the molecular dynamics simulation was run, using the Verlet algorithm. Since the actual simulation takes more than eight hours on a 386 PC with a floating point processor, the simulation was pre-run, and beginning, intermediate, and final structures were stored in a file library. The alpha helix was first heated to 100° C, and then allowed to denature. Structures from the