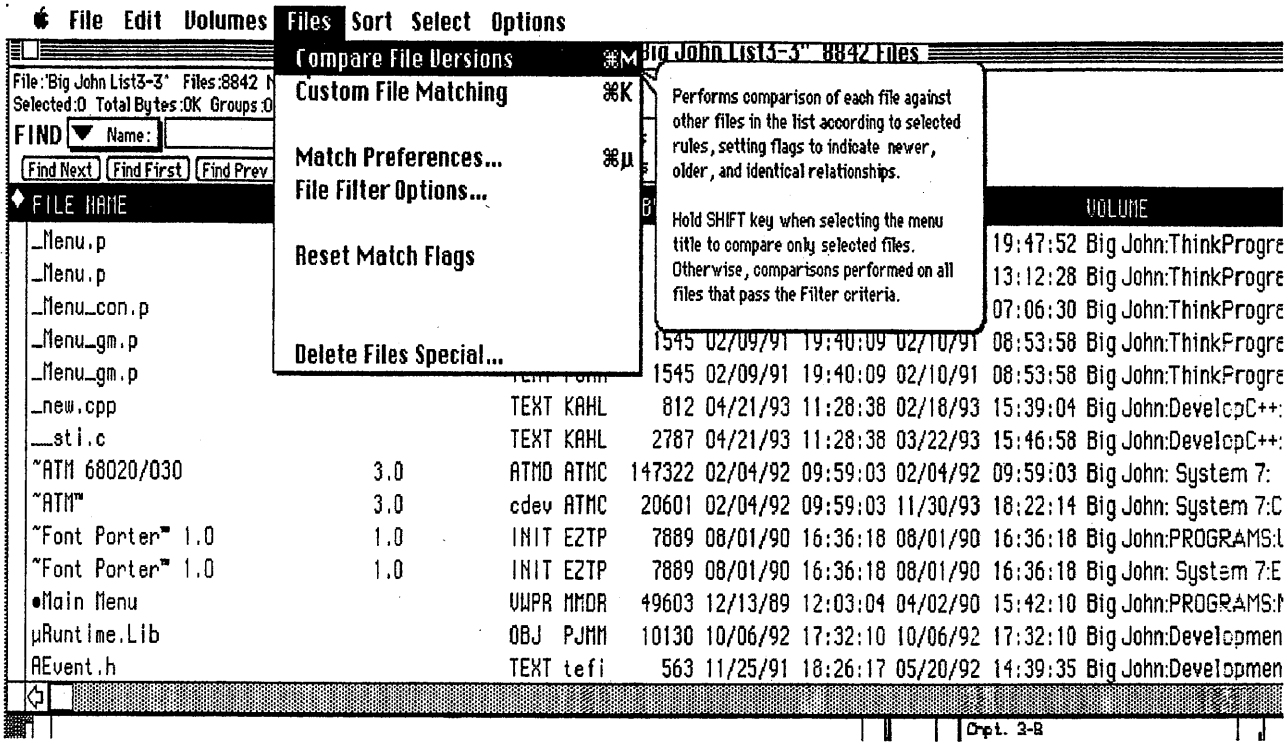

The utility includes balloon help shown above explaining one of the listings below the menu heading files.

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

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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

simulation were saved at 2.5 picosecond intervals for a period of 305 picoseconds. During the simulation, hydrogen bonds lengthened, and broke, and sometimes reformed. (A total of 122 structures).

Selected files (wire frame models) were viewed to determine what happened to the length of the hydrogen bonds that hold the helix together as the simulation progressed. The hydrogen bond lengths can be color-coded (1.8-1.9~ is red, 1.9-2.0~ is green, etc.) so that the changes in bond length are obvious.

Finally, a "movie" was constructed from all of the 122 structures that were saved from the simulation. (2) This "movie" may be stepped thru rapidly to provide an animated picture of the simulation. All of the individual structures may be examined. The animated version of the simulation destroys the student's picture of proteins as the rigid immobile structures that they see in text books.

REFERENCES 1. HHoweler, U., MOBY 1.5: Molecular Modelling on the PC. Springer- Verlag, New York, 1993.
2. The construction of a movie cannot be done with version 1.5 of MOBY. It requires version 1.6 which is currently in beta testing.

Stoichiometer

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Background

When you view yourself as a teacher, you focus your efforts on student learning. In chemistry teaching we expect students to acquire an array of skills. When confronted with a powerful tool like a desktop computer, the first thing a chemistry teacher would do is figure out ways to have that tool enhance student learning or improve the process of teaching. This is the history of computers in chemistry education over the last two decades.

When you view yourself as a chemist, you focus your efforts on chemistry. You seek computer tools that make old tasks simpler, better, easier, etc., and you seek to accomplish new tasks heretofore too difficult or tedious or otherwise prohibitive.

The teachers' goals focus on fixed targets, and the chemists' goals focus on moving those same targets. This became very clear to this writer — a teacher — in 1990. Similar situations apply to all of the professions. Professionals are accustomed to cognition based upon intracranial changes involving carbon atoms. We live in a world where much cognition is based upon intradevice changes involving silicon atoms, however.

Over a decade ago my physicist colleague Robert Fuller suggested to me that spreadsheets would change our approach to science. In 1987 I taught a workshop for high school teachers in which spreadsheets performed calculations typically covered in introductory chemistry. Teachers created the necessary spreadsheet cell formulas. I never really thought about having them give their students templates such that computations would be more automated. I came to the problem from the perspective of the traditional chemistry teacher.

Two kinds of very powerful software have changed my perspective. The symbolic mathematics programs that *do* calculus and algebra for me are quite remarkable. Really, the amount of time I spent learning that stuff — the tedium — contrasts markedly with a newly found ability to *play* with mathematics. Molecular structure programs subsume vast amounts of chemical knowledge and know how. Three cheers for the silicon atoms. How are teachers able to prepare students to understand chemistry, to use chemistry, and, for a few, to do chemistry in a world of silicon cognition?

Stoichiometry is at the heart of a modern, mainline course in general chemistry. We expect our students to be able to apply the mole concept in a wide variety of contexts, on paper and in the laboratory. Ever since 1988 I have fooled around with stoichiometry problems on HyperCard. Late in 1993, a new idea finally gelled for me — why not provide after-the-fact tutoring, retrospective tutoring, in a chemists' tool? Stoichiometer is a chemists' tool that does most of the stoichiometric tasks that we ask students to do. It includes essentially all of the tasks chemists actually do, the latter being more of a subset than a superset of the former. Stoichiometer removes much of the tedium of stoichiometry. It remembers — storing substances and reactions in clickable lists. It can import whole catalogs from vendors. It handles significant figures. But, unlike other tutorial materials, the user can enter *any* problem. Stoichiometer will try to solve that problem and provide feedback when it detects difficulties (like an unbalanceable equation, or diluting 0.6 M NaCl to get 6.0 M NaCl, or getting the gaseous volume of $CuSO_4(H_2O)_5$). Most important, in the absence of getting stuck trying to solve the problem, Stoichiometer will give context-specific feedback about how it solved its most recent problem.

A conventional path that a teacher might follow when using software would be to pose a problem that the student would attempt to solve using