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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 participa-
tion in our activities.



EDITOR

An interesting use of advanced graphics.

by Brian Pankuch,

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Princeton:

I arrived at the Art History class
just at the start of the lecture. Kirk
sat me down in front of the Sili-
con Graphics computer, toward the
back of the room. The lighting was
subdued, which made the 20" color
screen quite bright. The main rea-
son 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 profes-
sor of Art History, explained we were
to explore a database containing
high quality reproductions of paint-
ings, frescos, the buildings holding
the art, artists who made it, people
who commissioned 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 data-
base, 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. There were 7 students and
4 professors visiting from other uni-
versities and other departments at
Princeton.

Some followed step by step with
students generously helping visit-
ing 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 se-
verely under strength for RAM- a
mere 16 Meg. He feels they need at
least 32 Meg each locally while be-
ing 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 fres-
coes 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 realisti-
cally 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, com-
pared 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 stu-
dents 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 con-
tinue doubling the size of the pic-
ture, and to scroll through at great
magnification that allows me to see
details that Alice is putting into con-
text. Peter stays close to me be-
cause I keep exploring in all direc-
tions and crashing his neat inter-
face. 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 assign-

ment to answer a number of questions by exploring 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 History-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 over 10,000 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.

File Edit Volumes Files Sort Select Options

"Big John List3-3" 8842 Files •

File: 'Big John List3-3' (NOT saved) Files: 6842 Mem Used: 490K/2,579K (no match data) time: 0:02
Selected: 1 Total Bytes: 0K Groups: 0

FIND Name: [] Equals Includes
Find Next Find First Find Prev Find All Type: [] Creator: [] Begins Ends

FILE NAME	VERSION	TYPE	CREA	BYTES	CREATED	MODIFIED	VOLUME	PATH
Original Sail		PICT	ppxi	920510	09/01/91	01:52:36	12/06/91	18:21:25 Big John:PROGRAMS:Font stuff:Pictures:
Q & A index.inv		KRSI	HKRS	1004611	11/19/91	17:43:04	11/26/91	16:24:39 Big John:of Interest:Spinside Mac and Friends:Q & A Stack 4.0.4:Q & A kr
System copy	7.1	zsys	MACS	1098724	08/27/92	12:00:00	12/06/93	18:25:42 Big John: System 7:
MacInTax '93	V11.01	APPL	MIT3	1106456	01/15/94	15:00:00	01/15/94	15:00:00 Big John:MacTax copy:
MacInTax '93-2	V11.01	APPL	MIT3	1106456	01/15/94	15:00:00	01/15/94	15:00:00 Big John:MacTax:
MYM 5.0	5.0	APPL	MYMC	1143315	07/08/92	17:44:08	07/09/92	16:26:13 Big John:of Interest:MYM 5.0 Folder:
ChemIntosh3.3	3.3	APPL	CHYN	1150483	11/03/93	13:14:25	11/23/93	07:09:02 Big John:PROGRAMS:CHEM PROGRAMS:ChemIntosh3.3:
System	7.1	zsys	MACS	1172262	08/27/92	12:00:00	02/23/94	13:47:48 Big John: System 7:
MacroMind Director 3.0	3.0	APPL	MHDR	1196791	06/12/91	17:59:23	04/24/92	08:56:48 Big John:PROGRAMS:New MacroMind:
Toolbox Index Pages		Guid	DanR	1306649	12/17/92	23:11:53	12/17/92	23:37:58 Big John:PROGRAMS:THINK Reference f:
Learning Microsoft Excel		STAK	WILD	1348969	05/20/92	12:00:00	12/24/93	18:03:03 Big John:excel:
Excel Help		HELP	XCEL	1359106	05/20/92	12:00:00	12/24/93	18:00:18 Big John:excel:
Horton VolumeSaver Data		PNCv	PNfs	1521177	10/07/92	19:46:23	01/20/93	17:26:22 Big John:
Quicken 4	4	APPL	INTU	1527234	05/10/93	13:59:58	07/28/93	19:45:20 Big John:PROGRAMS:Quicken 4 Folder:
MACINTAX.HLP		MITH	MIT2	1613805	01/13/93	14:00:00	01/13/93	14:00:00 Big John:MacTax:Tax-for-92:Newest-for 92:Help Folder:
Tech Notes index.inv		KRSI	HKRS	1709157	10/14/91	16:39:22	11/26/91	16:24:39 Big John:of Interest:Spinside Mac and Friends:Technical Notes Stack:Te
System-old	7.1	zsys	MACS	1822862	08/27/92	12:00:00	02/14/94	18:27:58 Big John:System Stuff:
PageMaker 4.2	4.2	APPL	ALD4	1839263	12/18/91	14:18:57	12/18/91	14:18:14 Big John:PROGRAMS:Aldus PageMaker 4.2:
Q & A Stack 4.0.4		STAK	WILD	1873230	11/13/90	10:31:13	11/26/91	16:28:40 Big John:of Interest:Spinside Mac and Friends:Q & A Stack 4.0.4:
Excel	4.0	APPL	XCEL	1885091	05/08/92	08:24:08	12/24/93	17:59:07 Big John:excel:
RMED Dictionary III		RMH3	RMED	1935120	06/25/90	19:59:41	06/25/90	21:08:02 Big John: System 7:
MACINTAX.HLP		MITH	MIT3	2087227	01/15/94	15:00:00	01/15/94	15:00:00 Big John:MacTax copy:Help Folder:
MACINTAX.HLP		MITH	MIT3	2087227	01/15/94	15:00:00	01/15/94	15:00:00 Big John:MacTax:Help Folder:
Spinside index.inv		KRSI	HKRS	2565234	07/10/91	16:28:38	11/26/91	16:24:39 Big John:of Interest:Spinside Mac and Friends:Spinside Macintosh:SM in

File Edit Volumes Files **Sort** Select Options

File: 'Big John List3-3' (NOT saved) Files: 884
Selected: 1 Total Bytes: OK Groups: 0

FIND Name: []
Find Next Find First Find Prev Find All

FILE NAME VER

Disinfectant INIT	3
.o Converter	1
5 test	
BBarMin-93MM may	
BBarMin-93MM 11	
BeginProblem_M	
BeginProblem_M	
BigAndSmall	
BigAndSmall	
BigAndSmall	
BigAndSmall	
BigAndSmall SAVE	
BigAndSmall SAVE	
ButtonLine-93MM	
C. 10 TEST1	
C10 TEST2	
CHP 5A-test	
CHPT 5 Test 2	
chpt 7 test	
Chpt. 3-B	
CHPT. 5-B test	
chpt. 6-A test	
chpt. 8 test	
chpt. 8-A w.s.	

Files by selected (0 last) #1
Files by name #1
Files by match flags (0 last) #1
Files by version & name #4
Files by type (0 last) #4
Files by creator (0 last) #2
Files by size #2
Files by created #5
Files by modified #5
Files by volume (0 last) #3
Files by path (0 last) #3
Files by match index, flags & last #3

Volumes by selected
Volumes by name
Volumes by free
Volumes by total
Volumes by files
Volumes by created
Volumes by modified

MODIFIED	VOLUME	PATH
4 12/05/93 08:52:24	Big John: System 7: Extensions:	
1 05/01/93 12:09:17	Big John: DevelopC++: Symantec C++ for Macintosh: Translators:	
2 10/15/91 20:53:12	Big John: Word5: ellen.physical.science:	
4 09/07/93 07:07:24	Big John: ThinkPrograms: Marksman stuff: NEW Templates: sept93: Apr93:	
4 01/30/93 10:52:04	Big John: ThinkPrograms: Marksman stuff: BBProjects: Template:	
1 04/16/92 09:27:49	Big John: ThinkPrograms: OLD VERSIONS: Math: EXP FONTS: Proto:	
1 06/24/92 19:42:04	Big John: ThinkPrograms: OLD VERSIONS: Math: Proto: From other program	
6 06/03/93 08:38:11	Big John: ThinkPrograms: OLD VERSIONS: SigFig: PARTS copy:	
6 06/04/93 06:39:37	Big John: ThinkPrograms: OLD VERSIONS: Old SigFig: appl:	
6 06/03/93 19:22:15	Big John: ThinkPrograms: OLD VERSIONS: SigFig: PARTS:	
6 06/04/93 11:17:45	Big John: ThinkPrograms: SigFig May 1993: Proj: J:	
6 06/22/89 11:38:56	Big John: ThinkPrograms: OLD VERSIONS: Old SigFig: appl:	
6 06/22/89 11:38:56	Big John: ThinkPrograms: OLD VERSIONS: SigFig:	
4 01/14/93 17:59:54	Big John: ThinkPrograms: Marksman stuff: Junk?:	
0 03/04/90 20:58:32	Big John: Word5: ellen.CHEMISTRY:	
0 03/05/90 21:44:29	Big John: Word5: ellen.CHEMISTRY:	
4 10/15/91 20:47:33	Big John: Word5: ellen.physical.science:	
6 11/20/91 20:57:07	Big John: Word5: ellen.CHEMISTRY:	
4 06/24/90 17:27:24	Big John: Word5: ellen.physical.science:	
5 10/07/91 17:37:43	Big John: Word5: ellen.physical.science:	
6 06/21/90 16:04:56	Big John: Word5: ellen.physical.science:	
AWWP PS12 3589 06/24/90 17:30:04	06/24/90 17:30:04	Big John: Word5: ellen.physical.science:
AWWP PS12 4767 06/25/90 21:17:25	06/25/90 21:17:25	Big John: Word5: ellen.physical.science:
AWWP PS12 2518 06/24/90 17:33:47	06/24/90 17:33:47	Big John: Word5: ellen.physical.science:

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

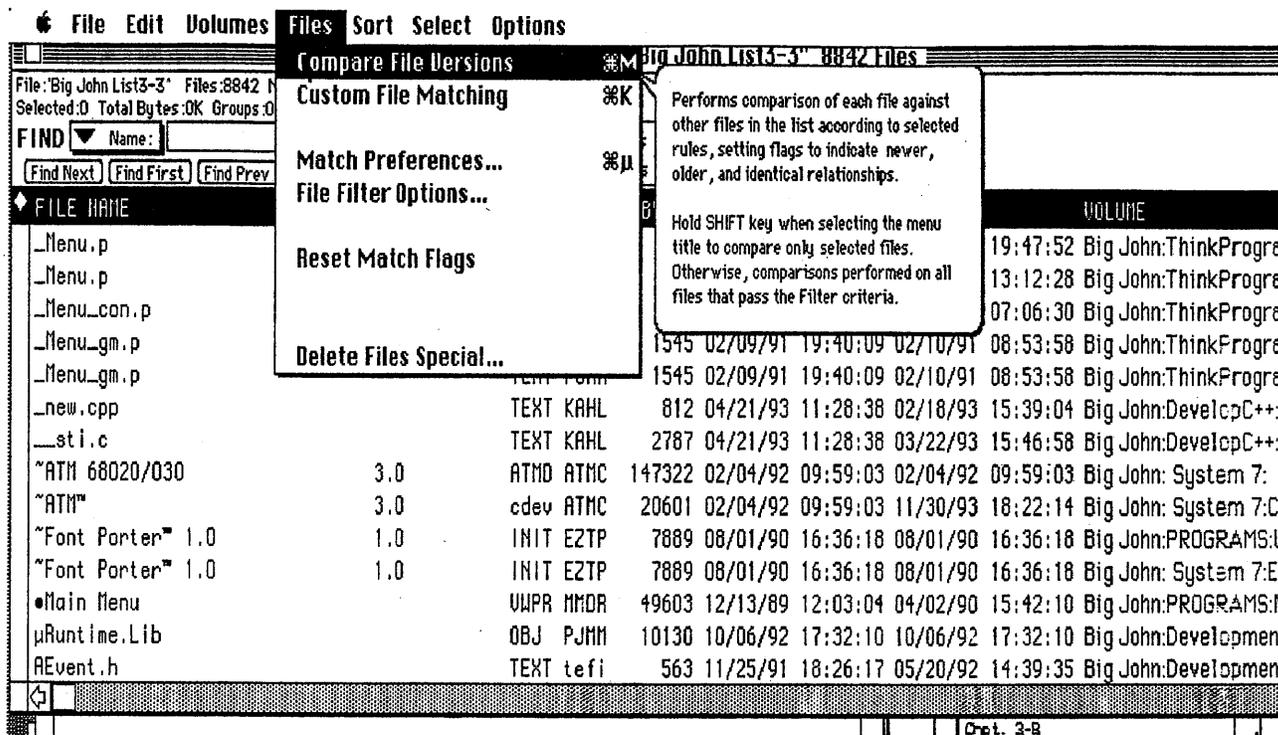
File Edit Volumes Files **Sort** Select Options

File: 'Big John List3-3' (NOT saved) Files: 8842 Mem Used: 490K/2,579K (no match data) time 0:03
Selected: 1 Total Bytes: OK Groups: 0

FIND Name: []
Find Next Find First Find Prev Find All Type: [] Creator: []
 Equals Includes
 Begins Ends

FILE NAME VERSION TYPE CREATOR BYTES CREATED MODIFIED VOLUME PATH

FILE NAME	VERSION	TYPE	CREA	BYTES	CREATED	MODIFIED	VOLUME	PATH
Disinfectant INIT	3.3	INIT	D2C1	7789	12/05/93 08:52:24	12/05/93 08:52:24	Big John: System 7: Extensions:	
.o Converter	1.0	TRAN	oCnv	40206	05/01/93 12:06:51	05/01/93 12:09:17	Big John: DevelopC++: Symantec C++ for Macintosh: Translators:	
5 test		AWWP	PS12	4332	11/05/90 22:18:12	10/15/91 20:53:12	Big John: Word5: ellen.physical.science:	
BBarMin-93MM may		grcP	grcE	33078	09/07/93 07:07:24	09/07/93 07:07:24	Big John: ThinkPrograms: Marksman stuff: NEW Templates: sept93: Apr93:	
BBarMin-93MM 11		grcP	grcE	48526	01/30/93 10:52:04	01/30/93 10:52:04	Big John: ThinkPrograms: Marksman stuff: BBProjects: Template:	
BeginProblem_M		TEXT	PJMM	69143	03/06/90 07:05:01	04/16/92 09:27:49	Big John: ThinkPrograms: OLD VERSIONS: Math: EXP FONTS: Proto:	
BeginProblem_M		TEXT	PJMM	69501	03/06/90 07:05:01	06/24/92 19:42:04	Big John: ThinkPrograms: OLD VERSIONS: Math: Proto: From other program	
BigAndSmall		TEXT	PJMM	51122	06/22/89 17:39:26	06/03/93 08:38:11	Big John: ThinkPrograms: OLD VERSIONS: SigFig: PARTS copy:	
BigAndSmall		TEXT	PJMM	52294	06/22/89 17:39:26	06/04/93 06:39:37	Big John: ThinkPrograms: OLD VERSIONS: SigFig: PARTS:	
BigAndSmall		TEXT	PJMM	51282	06/22/89 17:39:26	06/03/93 19:22:15	Big John: ThinkPrograms: OLD VERSIONS: SigFig: PARTS:	
BigAndSmall		TEXT	PJMM	51868	06/22/89 17:39:26	06/04/93 11:17:45	Big John: ThinkPrograms: SigFig May 1993: Proj: J:	
BigAndSmall SAVE		TEXT	PJMM	46170	04/28/89 18:46:26	06/22/89 11:38:56	Big John: ThinkPrograms: OLD VERSIONS: Old SigFig: appl:	
BigAndSmall SAVE		TEXT	PJMM	46170	04/28/89 18:46:26	06/22/89 11:38:56	Big John: ThinkPrograms: OLD VERSIONS: SigFig:	
ButtonLine-93MM		grcP	grcE	60362	01/14/93 17:59:54	01/14/93 17:59:54	Big John: ThinkPrograms: Marksman stuff: Junk?:	
C. 10 TEST1		AWWP	PS12	5223	03/04/90 20:58:30	03/04/90 20:58:32	Big John: Word5: ellen.CHEMISTRY:	
C10 TEST2		AWWP	PS12	5715	03/05/90 21:37:40	03/05/90 21:44:29	Big John: Word5: ellen.CHEMISTRY:	
CHP 5A-test		AWWP	PS12	4035	06/15/90 21:28:24	10/15/91 20:47:33	Big John: Word5: ellen.physical.science:	
CHPT 5 Test 2		AWWP	PS12	3999	11/20/91 20:57:06	11/20/91 20:57:07	Big John: Word5: ellen.CHEMISTRY:	
chpt 7 test		AWWP	PS12	4526	06/24/90 17:27:24	06/24/90 17:27:24	Big John: Word5: ellen.physical.science:	
Chpt. 3-B		AWWP	PS12	5121	06/02/90 15:20:25	10/07/91 17:37:43	Big John: Word5: ellen.physical.science:	
CHPT. 5-B test		AWWP	PS12	3992	06/21/90 16:04:56	06/21/90 16:04:56	Big John: Word5: ellen.physical.science:	
chpt. 6-A test		AWWP	PS12	3589	06/24/90 17:30:04	06/24/90 17:30:04	Big John: Word5: ellen.physical.science:	
chpt. 8 test		AWWP	PS12	4767	06/25/90 21:17:25	06/25/90 21:17:25	Big John: Word5: ellen.physical.science:	
chpt. 8-A w.s.		AWWP	PS12	2518	06/24/90 17:33:47	06/24/90 17:33:47	Big John: Word5: ellen.physical.science:	



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.wycc.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 understanding 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 polyaniline 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 polyaniline polymer was forced to assume the conformation of the template alpha helix.

Then the template was removed, and an energy minimiza-

tion was done on the polyaniline 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