Chemistry software hints

For help with SciFinder and other library related material, see this wonderful resource.

MestreNova is a wonderful tool for manipulating NMR files. The manual for 6.0.4 is here

For X-Ray Chrystalography analysis, we have installed apex2 on laue, the manual is can be downloaded.

You will need to login to laue: ssh -Y laue.coby.edu

and then type: apex &

to run it.

Gaussian is available on nscc, all 17 Macintosh in the schupf lab, and on all

wet lab imaged macs in Keyes. These macs run spartan remotely from schupflab over

an X windows connection. Under Mac OS you may need to install XQuartz.

http://www.ks.uiuc.edu/Training/Tutorials/Reference/macosxprimer.html

MOE short hints (PDF)

Gaussian 03 online manual is here, with Gaussian 09 here.

After you submit a job, that is going to take a while (>3 hour), you can quit out of gview. If you leave gview open, after the job is done, it uses on full cpu at 100%.
Personally I think this is a bug, but they don't.

Here is was top would report:

top - 13:37:20 up 63 days, 2:23, 3 users, load average: 8.40, 8.81, 8.95
Tasks: 215 total, 2 running, 213 sleeping, 0 stopped, 0 zombie
Cpu(s): 49.9%us, 0.3%sy, 49.8%ni, 0.0%id, 0.0%wa, 0.0%hi, 0.0%si, 0.0%st
Mem: 32502784k total, 2481692k used, 30021092k free, 36136k buffers
Swap: 2031608k total, 256k used, 2031352k free, 682076k cached
PID USER PR NI VIRT RES SHR S %CPU %MEM TIME+ COMMAND
21587 rhdowner 15 0 174m 40m 14m S 100.0 0.1 69:24.58 gview.exe

Spartan command line options:

spartan --help

```
--monitor            : Run the Spartan Monitor
--arch               : Display the CPU architecture of this machine
--submit [opt] <path> : Submit backend jobs
   --background
   --foreground
   --external-default-queue
   --external-queue <queue_name>
   --verbose <level>
--foreground-submit  : Submit backend jobs waiting for job to complete
--process-commands   : Process job command file
--unpack             : Unpack a .spartan file to Unix style format
--convert <old> <new> : Command line conversion utility
--select             : Return graphics mode
-inuse [-status]     : Inuse status
-inuse [add|-remove] : Modify inuse state
--library-path       : Print LD_LIBRARY_PATH
--root-path          : Print the spartan root path
--ldd                : Print the spartan GUI libary dependencies
```

--ldd-analysis <???> : Print module library dependencies
--ldd-so <lib???.so> : Print library dependencies

The following needs to be set to use mm3 in the schupflab:

add these two lines to your .cshrc

setenv MM32000ROOT /export/local/src
source $MM32000ROOT/mm32000/mm32000.cnf

An excellent resource for Varian Vnmr(j) can be found here.

If vnmrJ does not start correctly, close it, open a terminal and delete the lock file:

rm vnmrsys/lock*

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apex &

WebMO: available at http://schupflab.colby.edu/cgi-bin/webmo/login.cgi

you will need a login to use this service, check with rhdowner@colby.edu.

You may need to adjust your java settings (http://www.java.com/en/download/help/jcp_security.xml)

to anable http://schupflab.colby.edu   to dowloand and run the java based builder.