

Chem 09-560 Computational Chemistry

Using the CTC

Console login

At the console (in MI-320), login in by putting @psc.edu after your username:

```
User:      psc_username@psc.edu
password:  psc_password
```

Remote login

Note that the CTC machines do not accept telnet or ftp, you must use the secure commands ssh, scp etc.

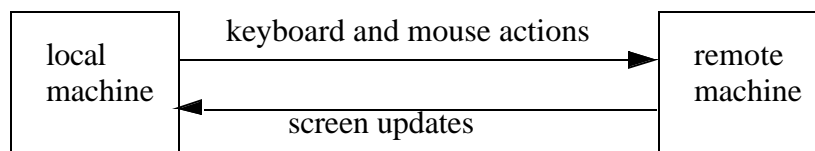
The CTC machines are named ctc#.psc.edu, where # is from 1 to 25. To login, do the following,

```
prompt> ssh psc_username@ctc#.psc.edu
```

and enter your psc password when asked.

Once you are logged on, type “who” to see if someone else is using the machine. If you are not the only person logged on, please log out and try another machine.

Setting your display for remote access



The local machine is the one you are sitting in front of. You must tell it that it is ok for the remote machine to update its screen:

```
xhost + remote_machine_name
```

You have to tell the remote machine to send all of its screen information to the local machine:

```
setenv DISPLAY local_machine_name:0.0
```

The 0.0 stands for the 0th screen on the 0th display device.

Setting up your local enviroment (choice 1)

You should type the following command to set your environment to something workable:

```
source /usr/skel/.cshrc
```

You will also need to enter the following:

```
alias cerius2 /afs/psc/projects/cerius/cerius2_3.5/bin/cerius2
```

Setting up your enviroment (choice 2)

You can also download the above commands as the file “ctc.cshrc” from the links page of the web site. Everytime you log on, you will need to type,

```
source ctc.cshrc
```

On your psc account, you can rename this file “.cshrc”, and then it will get run automatically everytime you long on. Do not, however, replace your andrew .cshrc file. If you do, you may break your account on andrew cluster machines.

Your path

When you type a command, the computer needs to know where to look for executable files. Your path is a list of directories the computer looks in to find these files. To see your path, along with other important configuration details, type:

```
set
```

Other important configuration information is held in the environment variables. You can see your environment variables by typing:

```
setenv
```

Using AFS to get access files

Both andrew and the PSC use AFS (formerly known as the andrew file system). This allows you access to your files from either system. Access is granted through *tokens*. To see your current tokens type:

```
tokens
```

If you are logged onto andrew, you should see an andrew token and the time at which it will expire. If you are logged into the ctc, you should see a psc token. (Problems occasionally arise with the ctc login script, and you may not automatically get a psc token when you log on. If this happens, you can manually as discussed next.)

To get a token for your files on andrew, type

```
klog andrew.cmu.edu
```

This will then prompt you for your andrew user name and id (user_id is sufficient, you do not need to enter user_id@andrew.cmu.edu). Similar, to get a token for your files on the psc, type

```
klog psc.edu
```

Configurations of CTC machines

TABLE 1. Memory available on CTC cluster machines

	Swap space (Mb)	RAM (Mb)	Disk space (total/avail)
CTC01**	428	96	8.3G/5.3G
CTC02*	428	96	2G/500M
CTC03***	340	160	2G/600M
CTC04*	328	96	2G/270M
CTC05***	428	160	8.3G/6.9G
CTC06***	428	160	8.3G/5.7G
CTC07*	403	96	1.9G/680M
CTC08*	404	96	1.9G/500M
CTC09***	428	160	3.9G/2.6G
CTC10*	403	96	2G/500M
CTC11*	340	96	2G/600M
CTC12***	928	160	4.1G/2.3G
CTC13*	350	96	2G/650M
CTC14**	428	96	2G/650M
CTC15*	398	96	1.5G/170M
CTC16*	352	96	1.1G/350M
CTC17	52	96	970M/130M
CTC18***	428	160	4.1G/2.4G
CTC19	50	96	974M/76M
CTC20*	401	96	2G/700M
CTC21***	428	160	4.1G/2.4G
CTC22*	301	96	1.5G/230M
CTC23	252	96	900M/70M
CTC24	428	64	8.3G/7.1G
CTC25*	352	96	2.1G/1.1G

RAM: Amount of physical memory in the computer. The command “`hinv`” (for hardware inventory) returns the amount of ram, and information on the processor and graphics subsystem.

Swap space: The operating system creates a memory space that consists of the RAM, and a “swap partition” on the hard-drive. If you use more memory than is available in RAM, the operating system will swap some of the memory out to the swap partition. If there is not enough room in the total memory space (RAM + swap) to hold a program or process, then that process can not be started. (Use `swap -ln` to get a report of the swap size). To run a mopac calculation in Cerius2, you need at least 300Mb of swap space.

Total disk space in machine (use `df -h`)