Running Simulations During the Afternoon Hands-on Sessions (revised!)

You will be running your simulations from the NAMD hands-on tutorial on Platinum, a cluster of dual-processor Pentium-III computers at NCSA. To make your life easier, we have provided a set of scripts which largely automate the process of transferring your files to and from Platinum, and running the simulation on Platinum.

1. Getting computer time on Platinum

Your first task during each afternoon session is to get computer time on the NCSA supercomputer called Platinum. During the afternoon sessions, you will have a dual-processor node on Platinum dedicated to you and you alone. This node is not available to you when you first log in to Platinum, however. To get to the node, first log in to Platinum, then type the following at the prompt:

~jphillip/SS03/runinter

(Note that that the character after the **SS** is a number 0, not the letter O.) This command may take a few minutes to complete, but when it does you will have a different-looking prompt, which tells you that you are now running what is known as an *interactive job* on Platinum. You will be able to use this node for six hours, or until you type **exit** at the command line. Once you leave the interactive session, you will need to run **runinter** again to get an interactive node again.

2. Your directory structure

After running the **tbss** script on the EWS machines, you will find yourself in a workspace directory. This is where you will be storing all your files, both the startup files for working through the tutorials as well as the output files from your structure building and simulation runs. Each hands-on tutorial will be contained in a subdirectory of this top-level workspace directory. Directions for getting the files for each tutorial will be provided separately. The important thing for transferring files is that each tutorial has a *unique directory name* in which all the files for that tutorial are to be found.

To be concrete, let's assume that the tutorial you're working on has a top level directory called *mytutorial*.

3. Copying files from EWS to Platinum

To copy the files you need to run on Platinum, you only need one command: **sendtopt**. You should be able to run this script whenever you're in the tbss environment (i.e., after you type *tbss* on the EWS machines). The way to use this command is as follows:

sendtopt *username directory*

Here, *username* means your username on Platinum, which is not necessarily the same as your username on the EWS machines. The second argument, *directory*, is the directory you want to copy to Platinum. **This directory must live in at the top of your tbss.work workspace directory.** So, for example, if my username on Platinum is *justin*, and the tutorial lives in a directory called namd-tutorial-files in the *tbss.work* directory, I could send files to Platinum by typing **sendtopt justin namd-tutorial-files**.

It doesn't matter what directory you're in when you type this command, and it doesn't matter how many times you type it: it will always copy just the files you need to run on Platinum. When you log in to Platinum, you will find a directory called *namd-tutorial-files* (for example) in your home directory, which will contain the files you need to run your jobs.

4. Running NAMD on Platinum

Once you are in an interactive node, you are ready to run a NAMD simulation. Go to the directory where the NAMD input files lives; let's say it's called *equil.conf*. Let's also say that you want the output file to be called *equil.log*. To run NAMD, use the following command:

~jphillip/SS03/tbnamd *inputfile logfile*

For this example, you would type *~jphillip/SS03/tbnamd equil.conf equil.log*. Note that you don't need to use the ">" character to redirect the output of NAMD to a file; **tbnamd** takes care of this for you.

To see the progress of your simulation, you can use *nedit* to view the output file. A better way to monitor progress while the simulation is running is to use the **tail** command. For example, to see continuous updates of the file *equil.log*, type the following at the prompt:

tail -f equil.log

When you want to stop monitoring, press Control-C. **tail** will not interfere with your simulation in anyway. Once the simulation is done, **tail** will not report any more updates, so if **tail** is still running you'll need to press Control-C to stop it.

5. Copying files from Platinum to EWS

To get files back from Platinum after your simulation is finished, use the **getfrompt** command. This command works exactly the same way as the **getfrompt** command:

getfrompt *username directory*

This command must be run from the EWS machines, not on Platinum. As before, *directory* is a directory in your *tbss.work* directory; for example, *namd-tutorial-files*. It will transfer just the new files you created in your simulation run back to EWS, so you can run it as many times as you need.