Four Ways to Run NAMD at SS03

There are now four different ways that you can run NAMD during the hands−on sessions. These new options may allow you to work more effectively, but *any method for running NAMD that you have been using should still work*. You don't need to try any of these if you don't want to!

On your local workstation

The same version of NAMD is installed on the Sun and Linux workstations as at NCSA. You can run NAMD, with reduced performance, on these machines if you have problems running jobs at NCSA or just to test config files. This may be useful during the evenings when we do not have dedicated nodes at NCSA. Use the tbnamd script to run NAMD on your local machine from the tbss> prompt:

tbss> **tbnamd *inputfile outputfile***

The job will start in the background and you can monitor it with the tail command:

tbss> **tail −f *outputfile***

Interactively at NCSA

First, log into the Platinum cluster using the NCSA username and password listed in your folder:

tbss> **ssh −l *ncsausername* pt.ncsa.uiuc.edu**

You are now be logged into one of the head nodes (with an "hn..." prompt). Next open an interactive job on one of the compute nodes:

hn03:~101% **~jphillip/SS03/runinter**

You should get a new "cn..." prompt in under two minutes, indicating that you are now logged into a compute node. If you don't, try again in a new window since a random error may have occurred. Use the cd command to change directories to the location of your files, and then you can run NAMD with the tbnamd script:

cn149:~101% **~jphillip/SS03/tbnamd *inputfile outputfile***

The job will start in the background and you can monitor it with the tail command:

cn149:~102% **tail −f *outputfile***

Batch jobs at NCSA

Running batch jobs gives you access to more processors, so your job will run in less time than it would in an interactive job. This is also a more efficient use of computational resources, because you only occupy the compute nodes when you are actually running NAMD. Log into your NCSA account on Platinum using ssh as described above, but *do not start an interactive job with the runinter script* . To submit a NAMD batch job, type:

hn03:~101% **~jphillip/SS03/runbatch *inputfile outputfile***

Your job will need to work it's way through the queueing system. In the afternoon sessions this should be only a couple of minutes, but in the evenings your job may wait in the queue for several hours. You can check the status of your job with the qstat command:

hn03:~102% **qstat −u *ncsausername***

The S column of the qstat output will show a Q while your job is waiting and an R when it is running. If you don't see your job listed at all after a minute, the job may have run and exited already, so check your output file. Once the job starts running you can monitor it with the tail command:

hn03:~103% **tail −f *outputfile***

Batch jobs through BioCoRE

Directions for running NAMD through BioCoRE are in your folder. Select the "TCB Special Queue" on Platinum with 4 processors in the afternoons and the "TCB Summer School" queue in the evenings.