NAMD

NAMD is a parallel, object-oriented molecular dynamics code designed for high-performance simulation of large biomolecular systems. NAMD scales to hundreds of processors on high-end parallel platforms and tens of processors on commodity clusters using switched fast ethernet. NAMD is file-compatible with AMBER, CHARMM, and X-PLOR.

NAMD is developed by the University of Illinois.

Usage

First you need to decide on the version of the software you want to use. Use

```
module avail namd
```

to check what versions are available. We normally recommend using the latest version available. For example, to load the version 2.9 of namd use

```
module load namd/2.9
```

For more details on using modules see our modules help guide.

NAMD is one of a few programs that may have a beta version installed. The beta version will have letter b in the version. For example, 2.10b1 is beta 1 version of 2.10. We do not recommend using beta versions, unless you really need to.

You must register your interest in NAMD with us to get access to it on the system. See Access Prerequisite section for more details.

A sample job script for NAMD is:

```
#!/bin/bash
PBS -l walltime=20:00:00
PBS -l mem=600MB
PBS -l ncpus=4
PBS -l software=namd
PBS -l wd
module load namd/2.9
mpirun -np $PBS_NCPUS namd2 configfile > output
```

The jobscript is then submitted to the queue using the qsub jobscript command.

Using the GPU queue

For namd versions 2.11 and 2.10.

namd2-gpu (openmpi)

```
module load namd/2.11
mpirun namd2-gpu input > output
```

namd2-node-gpu (multicore)

```
module load namd/2.11
namd2-node-gpu +p ${PBS_NCPUS} input > output
```

License requirements

To access NAMD you need to have registered at the Developer's website and let us know your username. The user registration page is linked through the archives so you will need to click an archive link (but you don't need to proceed to download as far as we're concerned). We are assuming that through the registration process you have read and agreed to the NAMD license agreement.

Once this is obtained, please request to join software group on https://my.nci.org.au if you wish to request access.

Note: that the registration process is the same as for VMD so if you have already registered for that you can provide those details.