

Introduction to Molecular Dynamics on ARCHER: Instructions for running parallel jobs on ARCHER

1 Introduction

This handout contains basic instructions for how to login in to ARCHER and submit jobs to the batch system. ARCHER is the UK's National HPC Service, and consists of a 118,080 core Cray XC30 system. For more detailed instructions, please refer to the ARCHER website:

<http://www.archer.ac.uk/documentation/>

2 Connecting to ARCHER via SSH

Each course participant has a numbered guest account (from `guest01` to `guest30`) - You should have been given a paper slip with your username on it. Please ensure you use the correct account for the duration of the course. The password will be given at the start of the practical session. To log in to ARCHER you should use the following details:

Server: `login.archer.ac.uk`

Username: `guestXX`

Password: *As provided*

For example, using the OpenSSH client on Linux or Mac run:

```
ssh guestXX@login.archer.ac.uk
```

You should see a welcome message, and obtain a command prompt on the ARCHER front-end similar to the following:

```
=====
login.archer.ac.uk
-----
```

```
This is a private computing facility. Access to this system is limited to those
who have been granted access by the operating service provider on behalf of the
issuing authority and use is restricted to the purposes for which access was
granted. All access and usage are governed by the terms and conditions of access
agreed to by all registered users and are thus subject to the provisions of the
Computer Misuse Act, 1990 under which unauthorised use is a criminal offence.
```

```
If you are not authorised to use this account then you must logout immediately.
-----
```

For assistance please contact the service helpdesk at: support@archer.ac.uk

```
=====
guest02@eslogin005:~>
```

If you have any difficulty connecting please ask the course staff.

For Windows, we recommend the PuTTY SSH client, which can be downloaded from:

<http://www.chiark.greenend.org.uk/~sgtatham/putty/>

3 Running a job

3.1 Filesystems

ARCHER uses the PBS batch processing system to schedule user jobs on the back-end nodes of the system. Please do not run compute-intensive tasks (e.g. NAMD or DL_POLY calculations) on the front-end nodes as these are shared by all users of the system.

ARCHER has two main file-systems, `/home/` and `/work/`. Upon login, you will be placed in your home directory on the `/home/` file system. This is intended for storage of files, code etc. It is not accessible to the back-end nodes where your jobs will run. `/work/` is a large, high-performance parallel file system, connected to the back-end nodes, and you should use this as a location to run your jobs from, store and access job input and output files.

To access your directory on `/work/` enter:

```
guest02@eslogin006:~> cd /work/y14/y14/guest02
guest02@eslogin006:/work/y14/y14/guest02>
```

Please note that data stored in the guest accounts will be erased shortly after the course ends. It is your responsibility to make copies of any data you wish to keep in another location before the course ends.

3.2 Module environment

Software is provided on ARCHER using the `module` command. You can see all the available modules by running `module avail`. For this course, you will need to load the following modules:

```
guest02@eslogin006:~> module load namd
```

The default version of `namd` on ARCHER is 2.9. To use the more recent version 2.10 load `namd/2.10` instead.

```
guest02@eslogin006:~> module load vmd
```

VMD running remotely on ARCHER may suffer from poor performance due to the network lag, and the lack of hardware 3D acceleration. You may prefer to run VMD on ARCHIE-WeSt via the ThinLinc client, or download and install it on your local machine from <http://www.ks.uiuc.edu/Research/vmd/>.

```
guest02@eslogin006:~> module load dlpoly
```

DL_POLY version 4.06 is loaded by default. DL_POLY Classic is also available by loading module `dlpoly/classic-1.9`.

3.3 Batch system

To run a job using the batch system, you must create a batch script containing the commands you wish to execute. An example script is below, please make a copy of it in your own directory:

```
guest02@eslogin006:/work/y14/y14/guest02> cat run.pbs
#!/bin/bash --login

#PBS -N test_job
#PBS -l select=1
#PBS -l walltime=0:5:0
#PBS -A y14

cd $PBS_O_WORKDIR

module load namd

aprun -n 24 namd2
```

The #PBS directives give the system information about your job, in this case that the job should be called test_job, that it should use 1 ARCHER node, and will run for up to 5 minutes. All jobs run during the course should use the y14 project account. You may edit these values if you wish to run on more nodes or for longer durations, before submitting the script.

Below this are a list of commands. The cd line ensures that the job runs correctly on the /work/ filesystem. A module is then loaded to give access to the NAMD software, and finally we launch the 'namd2' executable in parallel using 24 MPI processes. ARCHER has 24 processor cores per node, so when running your jobs make sure that the number of processors (-n 24) is less than 24 times the number of nodes (-l select=1).

Once the script has been created, we can submit the job using:

```
guest02@eslogin006:/work/y14/y14/guest02> qsub -q course1 run.pbs
230228.sdb
guest02@eslogin006:/work/y14/y14/guest02> qstat -u guest02
```

sdb:

Job ID	Username	Queue	Jobname	SessID	NDS	TSK	Req'd Memory	Req'd Time	Elap S	Time
230228.sdb	guest02	standard	test_job	--	1	24	--	00:05	Q	--

The qsub command submits the script, and returns a unique job ID. The qstat command can be used to monitor the status of the job. Q corresponds to a job which is waiting in the queue, R to a job which is running, and E to a job which is in the process of exiting. Once the job has completed it does not appear in the list.

The -q course1 argument refers to a Reservation ID 'course1' which has been set up to give exclusive access to a set of 15 nodes for the duration of the course. This should reduce queue waiting times. Please be aware this is shared by all participants so avoid running many jobs at one time, or using many nodes at once.

Note that jobs can still be run without the reservation ID, but will go into the main ARCHER queue along with all other jobs on the system, so will likely queue for (much) longer before running.

The standard output and error files produced by the job will be located in the current directory, and are numbered by the Job ID, alongside any additional files produced by NAMD :

```
guest02@eslogin006:/work/y14/y14/guest02> ls -ltr
```

```
total 8
-rw-r--r-- 1 guest02 y14 164 Apr 21 10:40 run.pbs
-rw----- 1 guest02 y14 0 Apr 21 10:52 test_job.e230228
-rw----- 1 guest02 y14 1523 Apr 21 10:52 test_job.o230228
```

In this case the standard output contains some information from the NAMD executable, followed by an error because no config file was provided. However, this is enough to show that the batch job worked as expected:

```
guest02@eslogin006:/work/y14/y14/guest02> cat test_job.o230228
...
Charm++> Running on MPI version: 3.0
Charm++> level of thread support used: MPI_THREAD_SINGLE (desired: MPI_THREAD_SINGLE)
Charm++> Running in non-SMP mode: numPes 24
Converse/Charm++ Commit ID: v6.5.1-rc2-2-g1bd45bf
Trace: traceroot: namd2
CharmLB> Load balancer assumes all CPUs are same.
Charm++> Running on 1 unique compute nodes (48-way SMP).
Info: NAMD CVS-2013-11-13 for CRAY-XC-MPI
Info:
Info: Please visit http://www.ks.uiuc.edu/Research/namd/
Info: for updates, documentation, and support information.
Info:
Info: Please cite Phillips et al., J. Comp. Chem. 26:1781-1802 (2005)
Info: in all publications reporting results obtained with NAMD.
Info:
Info: Based on Charm++/Converse 60500 for mpi-crayxc
Info: Built Mon Nov 18 11:19:00 GMT 2013 by namd on eslogin008
Info: Running on 24 processors, 24 nodes, 1 physical nodes.
Info: CPU topology information available.
Info: Charm++/Converse parallel runtime startup completed at 0.0171211 s
----- Processor 0 Exiting: Called CmiAbort -----
Reason: FATAL ERROR: No simulation config file specified on command line.
...
```

Congratulations, you have now run a simple NAMD job on ARCHER. Please proceed with the rest of the exercises. You will need to modify your batch script as necessary.

4 Visualisation & Analysis

To use VMD on ARCHER you will need to enable X11 forwarding in your SSH connection. With OpenSSH this is done by adding the `-X` flag. You will also need to load the `vmd` module before running VMD:

```
iains-mbp:~ ibethune$ ssh -X guest02@login.archer.ac.uk
```

```
Password:
```

```
Last login: Mon Apr 21 09:56:27 2014 from <snip>
```

```
=====  
login.archer.ac.uk  
-----
```

```
<snip>
```

```
=====  
guest02@eslogin005:~> cd /work/y14/y14/guest02
```

```
guest02@eslogin005:/work/y14/y14/guest02> module load vmd
```

```
guest02@eslogin005:/work/y14/y14/guest02> vmd geopt-pos-1.xyz
```

For plotting data, ARCHER has the following tools installed:

- GNUplot: simply type `gnuplot`
- XMGrace: first load the `xmgrace` module then run `xmgrace`