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Pulling it all together - Preparing, submitting and monitoring a job on Prince

In this section we will prepare, submit and monitor a small Amber (molecular dynamics) job. Our test case comes from the test suite that comes with Amber.

**Exercise**
Start a terminal session on Prince and replicate this example in it.

**Choose your own example**
After - or instead of - following this example through, prepare and submit a run of something genuinely relevant to your research. This way, if you are doing this tutorial in a classroom, the presenter will be available should you have questions or strike difficulties.

We're using Amber, so first we'll look for available modules. On Prince:
There's quite a few versions there. We'll select a recent one - and purge first to ensure we start from a clean environment

```
$ module purge
$ module list
No Modulefiles Currently Loaded.
$ module load amber/openmpi/intel/16.06
```

Take a look at what it did:

```
$ module list
Currently Loaded Modulefiles:
    1) centos/7          5) hdf5/intel/1.10.0p1         9) pnetcdf/openmpi/intel/1.6.0
    2) python/intel/2.7.12 6) netcdf/intel/4.4.1.1       10) amber/openmpi/intel/16.06
    3) cuda/8.0.44        7) intel/17.0.1
    4) zlib/intel/1.2.8   8) openmpi/intel/2.0.1
```

... clearly, Amber uses a lot of other packages. The modulefile has looked after loading the correct ones.
Loading the module set a useful environment variable, AMBERHOME. We’ll get our test case from there:

```bash
$ ls $AMBERHOME/test/amoeba_jac/
amoeba_jac.ips.mdot.save
amoeba_jac.mdout.save
amoeba_jac.pmemd.mdot.save
inpcrd
inpcrd.rst7
prmtop
Run.amoeba_jac
Run.amoeba_jac.ips
Run.amoeba_jac.pmemd
```

We are interested in the files highlighted in blue. Make a directory in your $HOME and copy them there.

`Run.amoeba_jac` is a script for running the test after building Amber - it’s not exactly what we want, but we’ll take some parts of it. First, we need the namelist file it creates, so we’ll cut-and-paste the lines between "cat > mdin <<EOF" and "EOF" into a file called "mdin". (Note the liberal use of shortcuts in the snapshot below. The TAB key is also useful here!)

```bash
$ mkdir $HOME/tutorial-2-ex1
$ cd !$
$ cp $AMBERHOME/test/amoeba_jac/[ip]* .
$ cp $AMBERHOME/test/amoeba_jac/Run.amoeba_jac .
$ cp Run.amoeba_jac mdin
$ vi mdin
# ... and selectively delete the unwanted lines
```

It should come out looking like this: (don’t worry about the blue text just yet)
Next we need to write a job script.

What resources will we need?

- It's a serial job, so nodes=1 and ntasks=1
- This test uses about 800MB of memory. We'll request 1GB to be sure
- The test takes less than a minute. We'll request 5 minutes and you can optionally increase the run length (currently 10 fs) by increasing \texttt{nstlim} in the \texttt{mdin} file (that blue text above).

As for the workflow, the script needs to:

- Load the Environment Module for Amber
- Set up a run directory. We'll run in \texttt{$SCRATCH$}, even though this is a very small test
  - \textbf{NOTE:} currently \texttt{$SCRATCH$} is only defined for login (usually just interactive) shells. We can make any shell a login shell (even if not interactive) by calling \texttt{bash} (or \texttt{csh}) with the \texttt{-l} option. See the first line of the script below.
  - copy the input files there
- Change into the run directory and run the job
  - The command to start this Amber job can be determined from the script \texttt{Run.amoeba_jac}:
    \begin{verbatim}
    sander -O -i mdin -o amoeba_jac.mdout
    \end{verbatim}
  - We can get a report at the end of the run on the time and memory resources used by using the \texttt{"time"} command.
    Here we give it an explicit path because bash has a builtin function called \texttt{"time"}, and we want the more powerful command from \texttt{/usr/bin}.
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --mem=1GB
#SBATCH --time=5:00

module purge
module load amber/openmpi/intel/16.06

# make a unique directory (by using the PBS job id in its name)
# The /*/ shortens the job id to the part before the first ".", see
# the "Parameter expansion" section of "man bash" for more
RUNDIR=${SCRATCH}/sbatch_amber_tut.${SLURM_JOB_ID/.*/}
mkdir $RUNDIR

# copy the input data from where we placed in in $HOME to the $RUNDIR
cd $RUNDIR
cp $SLURM_SUBMIT_DIR/inpcrd .
cp $SLURM_SUBMIT_DIR/prmtop .
cp $SLURM_SUBMIT_DIR/mdin .

# the command to start the simulation is:
# sander -O -i mdin -o amoeba_jac.mdout
# we can get timing and resource use information by running a command or program via
# "time":
# /usr/bin/time -v will report the time and memory used afterwards
/usr/bin/time -v sander -O -i mdin -o amoeba_jac.mdout

Finally, we can submit our job, and monitor its progress:

$ sbatch my_job_script.s

You'll get a job id returned.

Is it running yet?

$ squeue -u $USER

You could watch the output in the run directory:

$ ls -l ${SCRATCH}

Look for a directory whose suffix is the job id. Inside it, a file called amoeba_jac.mdout will be growing, with the output of the Amber run.

Finally, when the job finishes, you should see a slurm-*.out file in the directory you submitted from.

$ ls -lt
-rw-rw-r-- 1 johd johd 766 Jan 20 14:35 slurm-12418.out

Use 'cat' to see what is in the .out file. It's the timing information from /usr/bin/time -v. The job was very short! Try increasing nstlim (as mentioned above) so the job will take at least two or three minutes.

**Exercise**

Experiment with sbatch options for the job name, output and error file merging and location, resource limits (what if the job exceeds them? You might need to increase nstlim quite a lot to hit a resource limit).