## Putting all pieces together

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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:
$ module avail amber

----------------------------------------- /share/apps/modulefiles
-----------------------------------------
  amber/openmpi/intel/16.06

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.mdout.save
  amoeba_jac.mdout.save
  amoeba_jac.pmemd.mdout.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 `nstlim` in the `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 `$SCRATCH`, even though this is a very small test
  - NOTE: currently `$SCRATCH` is only defined for login (usually just interactive) shells. We can make any shell a login shell (even if not interactive) by calling bash (or csh) with the `-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 `Run.amoeba_jac`:
    ```bash
    sander -O -i mdin -o amoeba_jac.mdout
    ```
  - We can get a report at the end of the run on the time and memory resources used by using the "time" command. Here we give it an explicit path because bash has a builtin function called "time", and we want the more powerful command from `/usr/bin`

```
short md, nve ensemble
&cntrl
ntx=1, irest=0,
nstlim=10,
ntpr=1, ntwr=10000,
dt=0.001, vlimit=10.0,
cut=8., jfastw=4,
rtt=1, temp0=50.0, tempi=0.0,
iameoba=1,
/
&ewald
nfft1=80,nfft2=80,nfft3=80,
skinnb=2,nbtell=0,order=5,ew_coeff=0.45,
/
&amoeba
do_bond=1,do_ureyb=1,do_reg_angle=1,do_trig_angle=1,
do_opbend=1,do_torsion=1,do_pi_torsion=1,do_strbend=1,
do_torsion_torsion=1,do_amoeba_nonbond=1,
dipole_scf_tol = 0.01,dipole_scf_iter_max = 20,
sor_coefficient = 0.7,ee_damped_cut = 4.5,ee_dsum_cut = 6.7,
beeman_integrator=1,
/
```
#!/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).