Putting all pieces together - an R example

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Running jobs on the Prince Cluster

Accessing the Prince Cluster

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Software and Environment Module

Job script and resource request

- Introduction to job scheduling
- Submitting jobs with sbatch
- Requesting resources
- Using computing nodes interactively

Monitoring batch jobs

- Monitoring batch jobs - squeue
- What is running and where? slurmtop

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Putting all pieces together

- An Amber example
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Summary

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

In this section we will prepare, submit and monitor a small R job. Our test case comes from the NYU Data Services “Introduction to R” tutorial

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 R, so first we'll look for available modules. On Prince:

```
$ module avail r
--------------------------------------------- /share/apps/modulefiles ---------------------------------------------
gstreamer/intel/1.10.2   mothur/intel/1.35.1   r/intel/3.3.2
```

There's a few modules starting with r, and a couple of versions of R. We'll use the latest version, 3.1.2.

```
$ module purge
$ module list
No Modulefiles Currently Loaded.
$ module load r/intel/3.3.2
```

Take a look at what it did:

```
$ module list
Currently Loaded Modulefiles:
  1) jdk/1.8.0_111   2) intel/17.0.1   3) openmpi/intel/2.0.1   4) r/intel/3.3.2
```

... clearly, R uses a lot of other packages. The modulefile has looked after loading the correct ones.

```
$ module show r/intel/3.3.2
-------------------------------------------------------------------------------------------
/share/apps/modulefiles/r/intel/3.3.2.lua:
-------------------------------------------------------------------------------------------
whatis("R: a language and environment for statistical computing and graphics")
whatis("Name: r version: 3.3.2 compilers: intel")
load("intel/17.0.1")
load("jdk/1.8.0_111")
load("openmpi/intel/2.0.1")
prepend_path("MANPATH","/share/apps/r/3.3.2/intel/share/man")
prepend_path("PATH","/share/apps/r/3.3.2/intel/bin")
prepend_path("LD_LIBRARY_PATH","/share/apps/r/3.3.2/intel/lib64/R/lib")
prepend_path("PKG_CONFIG_PATH","/share/apps/r/3.3.2/intel/lib64/pkgconfig")
setenv("R_ROOT","/share/apps/r/3.3.2/intel")
setenv("R_INC","/share/apps/r/3.3.2/intel/lib64/R/include")
setenv("R_LIB","/share/apps/r/3.3.2/intel/lib64/R/lib")
family("R")
```

For our example, we'll get some code and data from /share/apps/examples:

```
$ mkdir /beegfs/$USER/R-example
$ cd !
$ cp /share/apps/examples/r/basic/* .
```

Take a look at the job script:
There are a few steps we can try here:

1. Start an interactive batch session, and run the example.R script interactively
2. Close the interactive session, and submit the batch script as a job:

   $ sbatch my_R_job.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}/R-example

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

**Exercise**

Experiment with sbatch options for the job name, output and error file merging and location, resource limits.