Using BU’s Shared Computing Cluster (SCC)

PY502

09/08/2023

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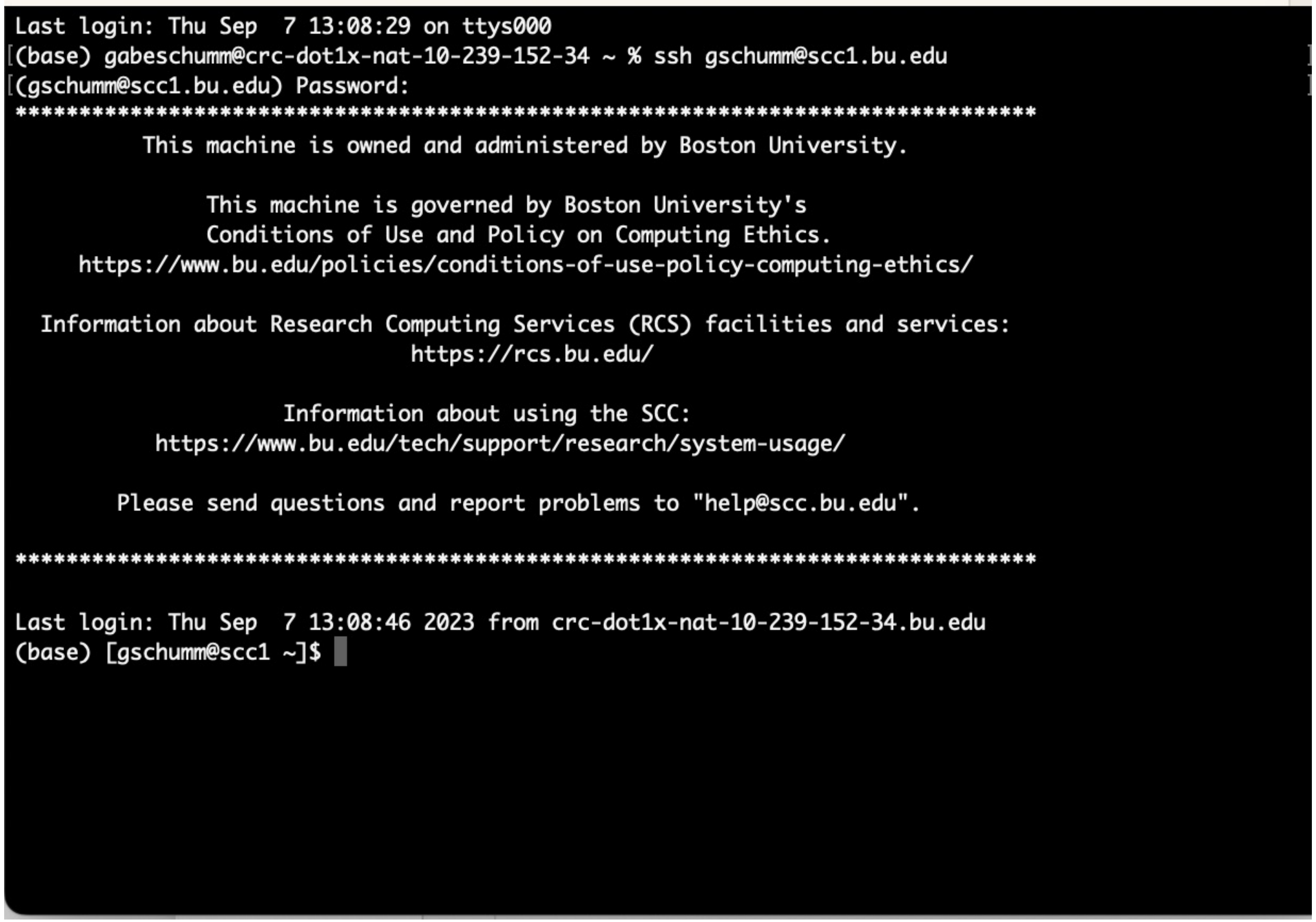
Options

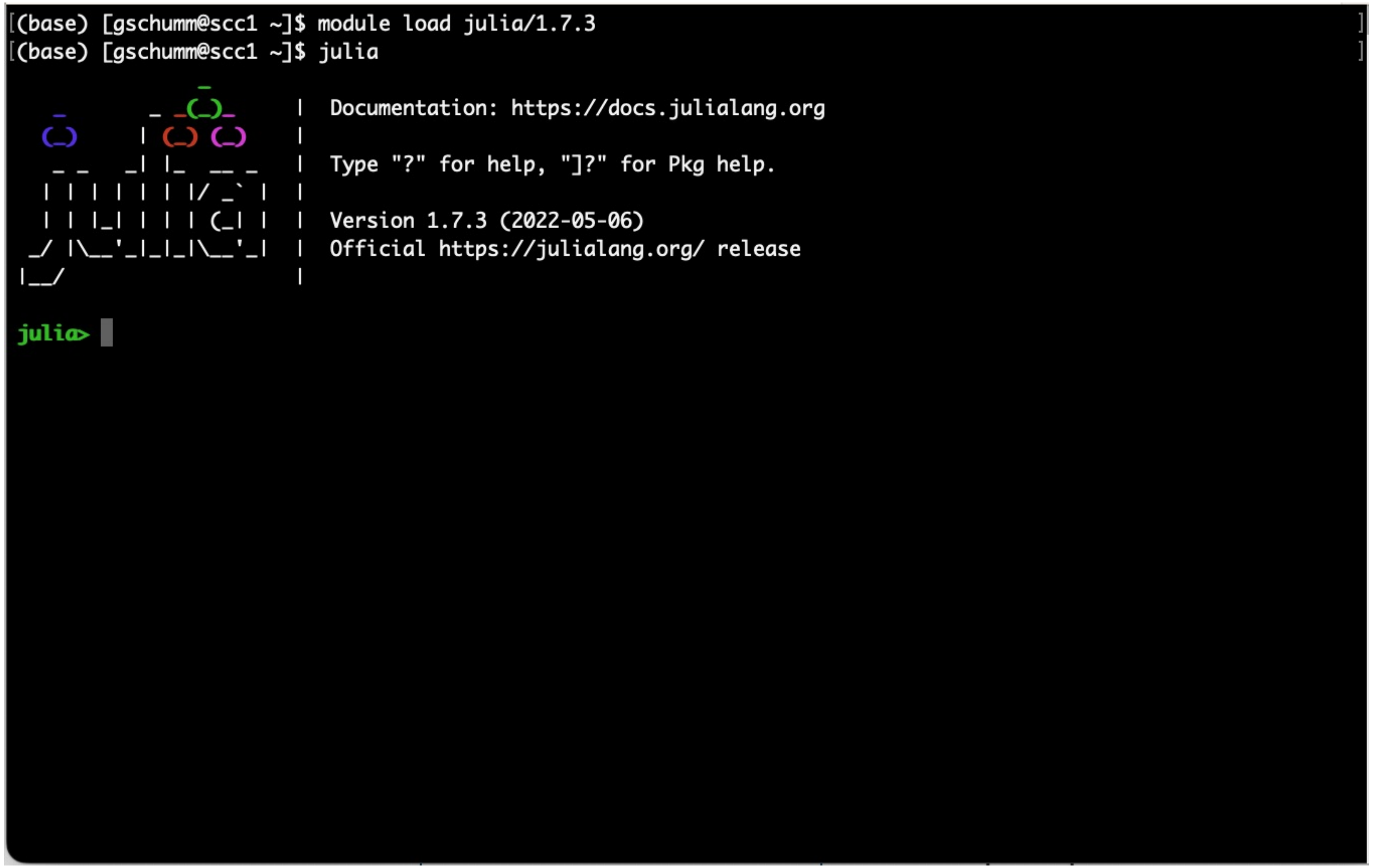
- Run code locally on your personal computer
  - Requires Julia be installed
  - Some homework assignments require substantial computing time
- Run code on the SCC as an *interactive job*
  - "suitable for code development and debugging"
  - **Ju**pyter notebooks
  - Dependencies already installed (for the most part)
  - Not recommended if code takes longer than a few minutes
- Run code on the SCC as a *batch job*
  - Best practice is to run (bug-free) code as batch job
  - Dependencies already installed (for the most part)

Setting up Julia



```
Last login: Thu Sep  7 13:08:29 on ttys000
[(base) gabeschumm@crc-dot1x-nat-10-239-152-34 ~ % ssh gschumm@scc1.bu.edu
[(gschumm@scc1.bu.edu) Password:
********************************************************************************
          This machine is owned and administered by Boston University.

               This machine is governed by Boston University's
               Conditions of Use and Policy on Computing Ethics.
     https://www.bu.edu/policies/conditions-of-use-policy-computing-ethics/

  Information about Research Computing Services (RCS) facilities and services:
                               https://rcs.bu.edu/

                     Information about using the SCC:
           https://www.bu.edu/tech/support/research/system-usage/

        Please send questions and report problems to "help@scc.bu.edu".

********************************************************************************

Last login: Thu Sep  7 13:08:46 2023 from crc-dot1x-nat-10-239-152-34.bu.edu
(base) [gschumm@scc1 ~]$ 
```

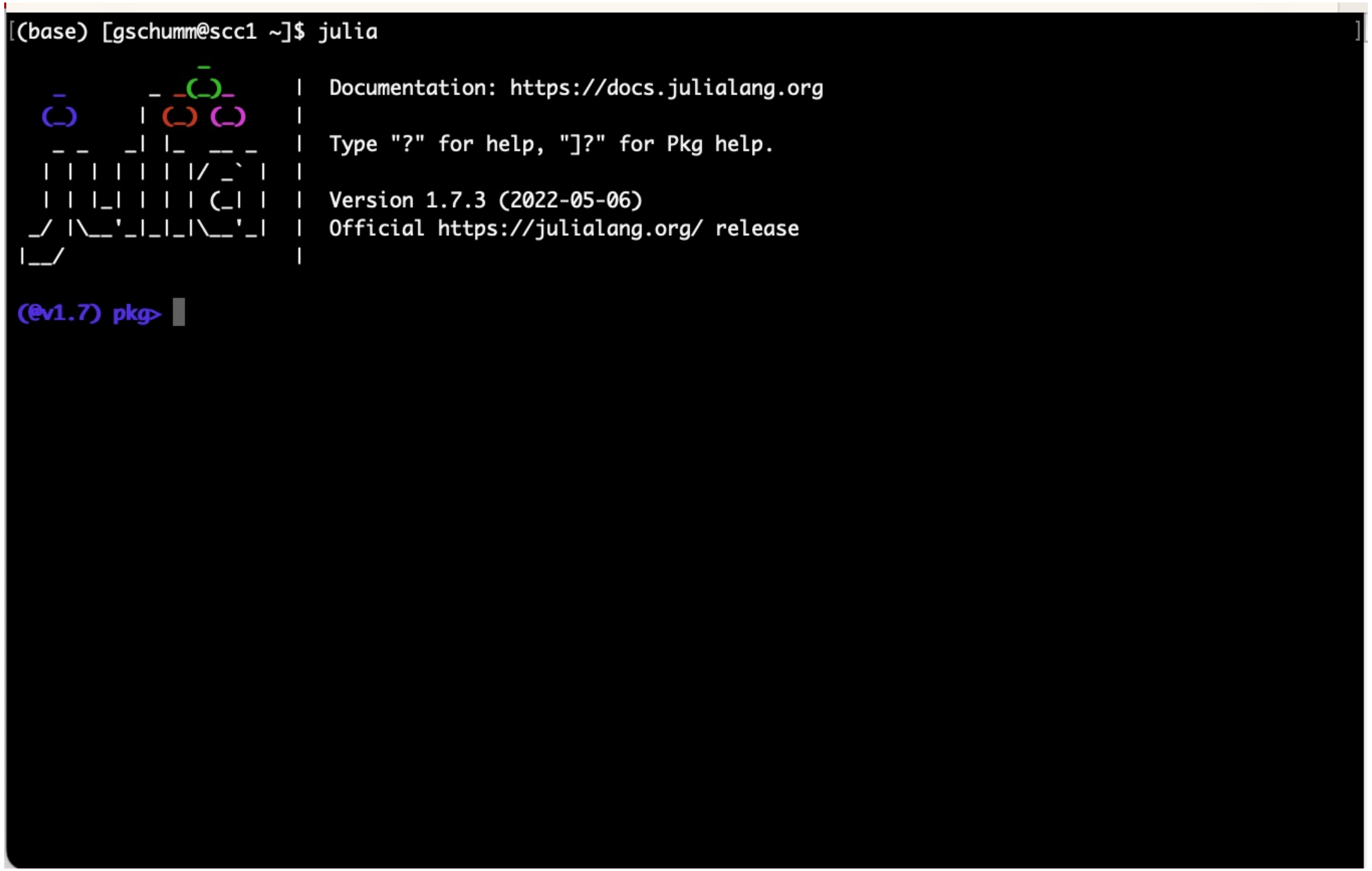
Setting up Julia



```
[(base) [gschumm@scc1 ~]$ module load julia/1.7.3
[(base) [gschumm@scc1 ~]$ julia
               _
   _       _ _(_)_     |  Documentation: https://docs.julialang.org
  (_)     | (_) (_)    |
   _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 1.7.3 (2022-05-06)
 _/ |\__'_|_|_|\__'_|  |  Official https://julialang.org/ release
|__/                   |

julia>
```

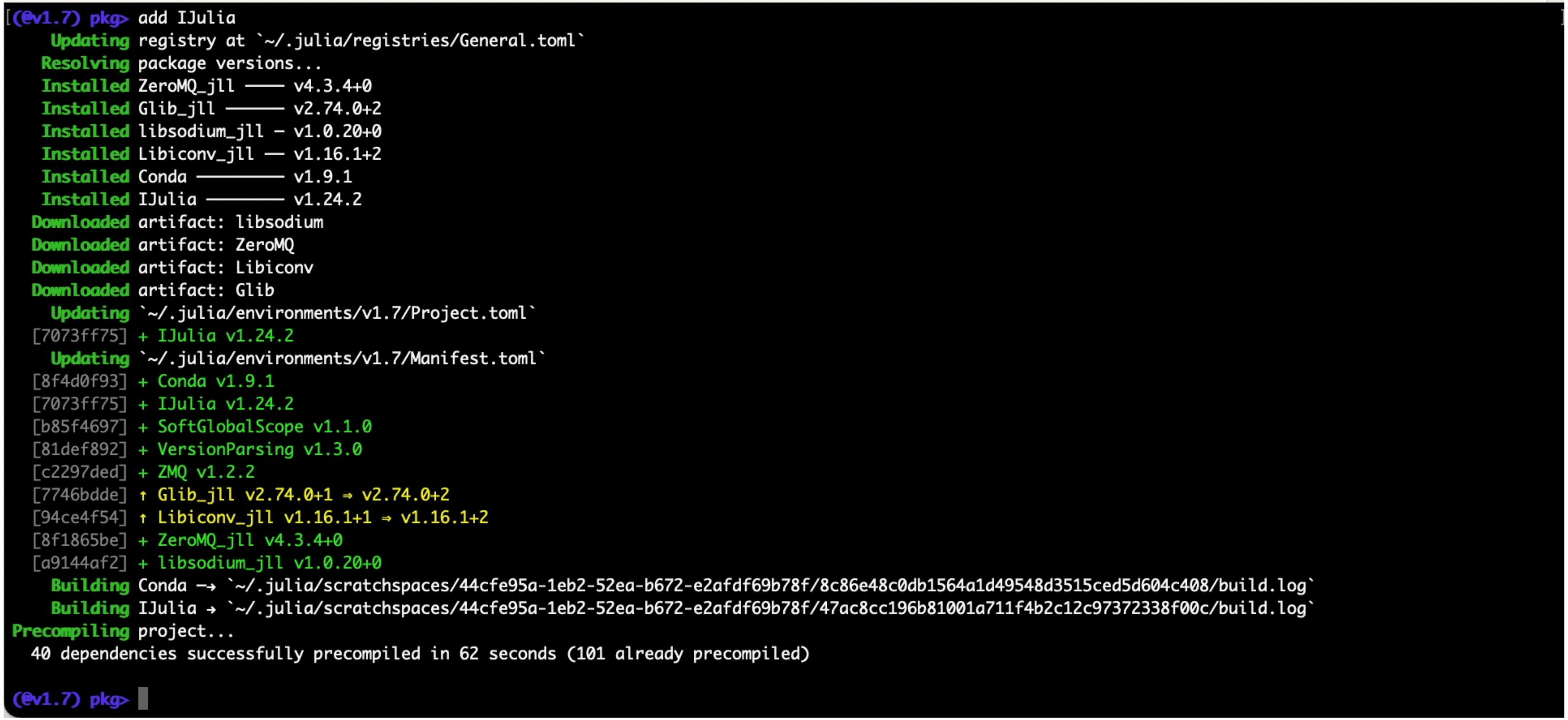
Setting up Julia

Type “]” to enter “Pkg REPL”



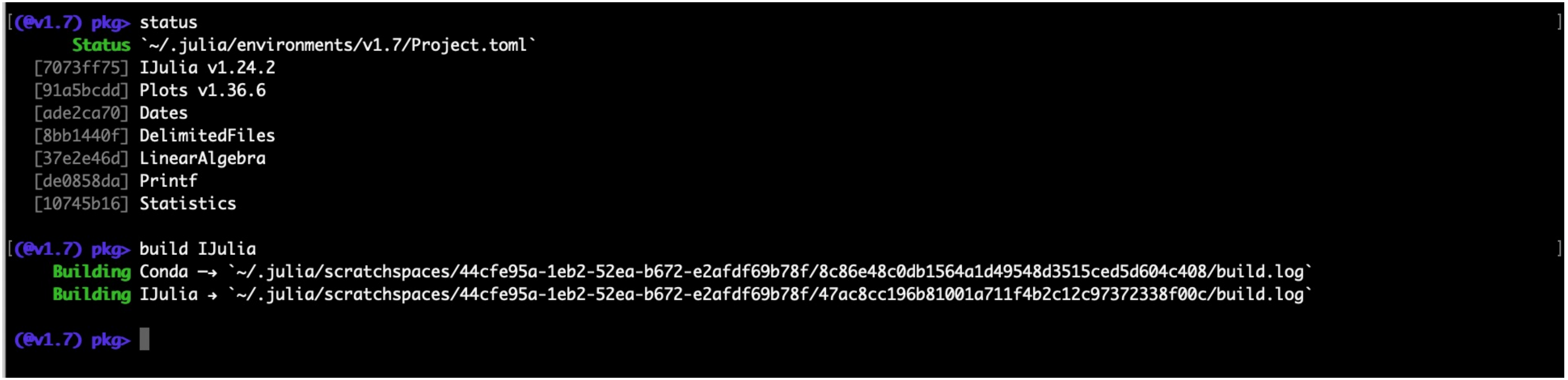
```
(base) [gschumm@scc1 ~]$ julia
               _
   _       _ _(_)_     |  Documentation: https://docs.julialang.org
  (_)     | (_) (_)    |
   _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 1.7.3 (2022-05-06)
 _/ |\__'_|_|_|\__'_|  |  Official https://julialang.org/ release
|__/                   |

(@v1.7) pkg>
```

Setting up Julia



```
[(@v1.7) pkg> add IJulia
    Updating registry at `~/.julia/registries/General.toml`
   Resolving package versions...
   Installed ZeroMQ_jll ──── v4.3.4+0
   Installed Glib_jll ────── v2.74.0+2
   Installed libsodium_jll ─ v1.0.20+0
   Installed Libiconv_jll ── v1.16.1+2
   Installed Conda ───────── v1.9.1
   Installed IJulia ──────── v1.24.2
  Downloaded artifact: libsodium
  Downloaded artifact: ZeroMQ
  Downloaded artifact: Libiconv
  Downloaded artifact: Glib
    Updating `~/.julia/environments/v1.7/Project.toml`
  [7073ff75] + IJulia v1.24.2
    Updating `~/.julia/environments/v1.7/Manifest.toml`
  [8f4d0f93] + Conda v1.9.1
  [7073ff75] + IJulia v1.24.2
  [b85f4697] + SoftGlobalScope v1.1.0
  [81def892] + VersionParsing v1.3.0
  [c2297ded] + ZMQ v1.2.2
  [7746bdde] ↑ Glib_jll v2.74.0+1 ⇒ v2.74.0+2
  [94ce4f54] ↑ Libiconv_jll v1.16.1+1 ⇒ v1.16.1+2
  [8f1865be] + ZeroMQ_jll v4.3.4+0
  [a9144af2] + libsodium_jll v1.0.20+0
    Building Conda ─→ `~/.julia/scratchspaces/44cfe95a-1eb2-52ea-b672-e2afdf69b78f/8c86e48c0db1564a1d49548d3515ced5d604c408/build.log`
    Building IJulia → `~/.julia/scratchspaces/44cfe95a-1eb2-52ea-b672-e2afdf69b78f/47ac8cc196b81001a711f4b2c12c97372338f00c/build.log`
 Precompiling project...
  40 dependencies successfully precompiled in 62 seconds (101 already precompiled)

(@v1.7) pkg> 
```

Setting up Julia



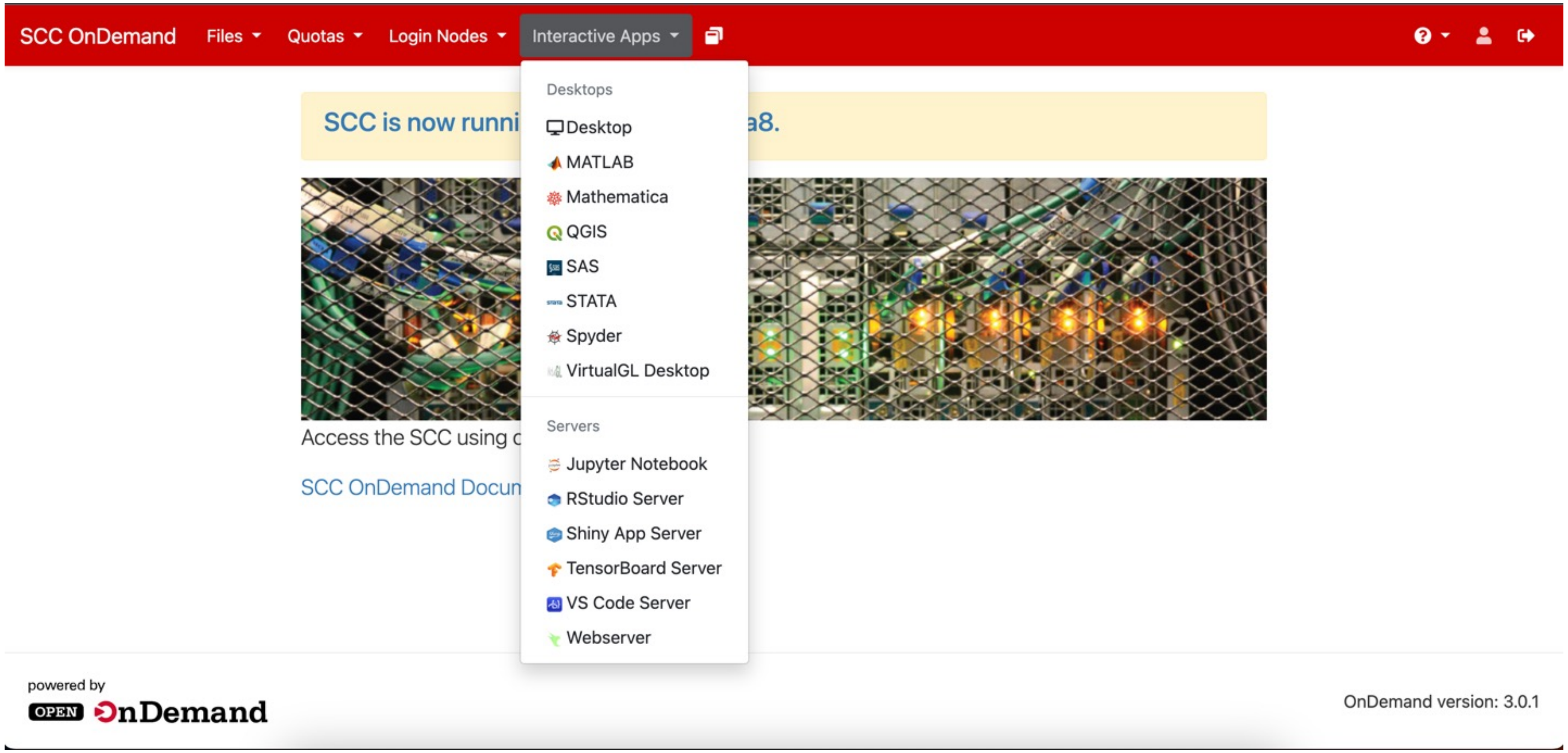
```
[(@v1.7) pkg> status
      Status `~/.julia/environments/v1.7/Project.toml`
  [7073ff75] IJulia v1.24.2
  [91a5bcdd] Plots v1.36.6
  [ade2ca70] Dates
  [8bb1440f] DelimitedFiles
  [37e2e46d] LinearAlgebra
  [de0858da] Printf
  [10745b16] Statistics

[(@v1.7) pkg> build IJulia
    Building Conda ─→ `~/.julia/scratchspaces/44cfe95a-1eb2-52ea-b672-e2afdf69b78f/8c86e48c0db1564a1d49548d3515ced5d604c408/build.log`
    Building IJulia → `~/.julia/scratchspaces/44cfe95a-1eb2-52ea-b672-e2afdf69b78f/47ac8cc196b81001a711f4b2c12c97372338f00c/build.log`

 (@v1.7) pkg> 
```

Useful Packages

- ”Plots”
- “Statistics”
  - mean, std
- “LinearAlgebra”
  - All matrix operations (eigvals/vecs, determinant, trace, etc.)
- ”DataFrames”
  - Like pandas in Python
  - Excel-like visualization/manipulation of tabular data
- ”DelimitedFiles”
  - Read and write tabular data
- “Printf”
  - Easier string formatting
  - `filename = @sprintf("p%02i.csv",3)` → `p03.csv`

Interactive Jobs

- OnDemand – access the SCC via your browser
- https://scc-ondemand1.bu.edu/

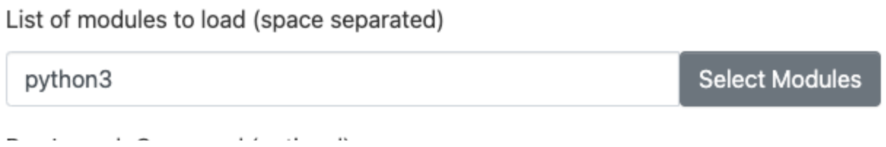


SCC is now runni a8.

Access the SCC using c

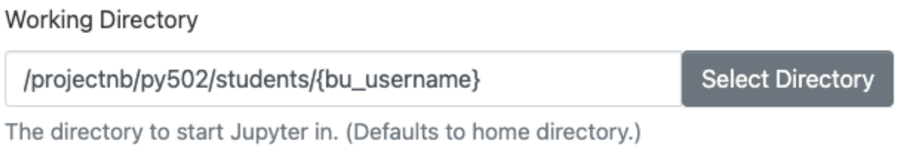
SCC OnDemand Docun

Jupyter Notebook



List of modules to load (space separated)

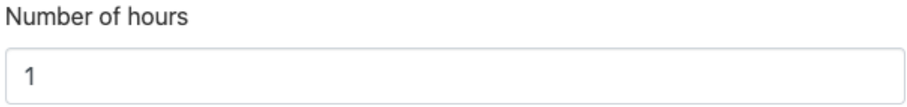
python3



Working Directory

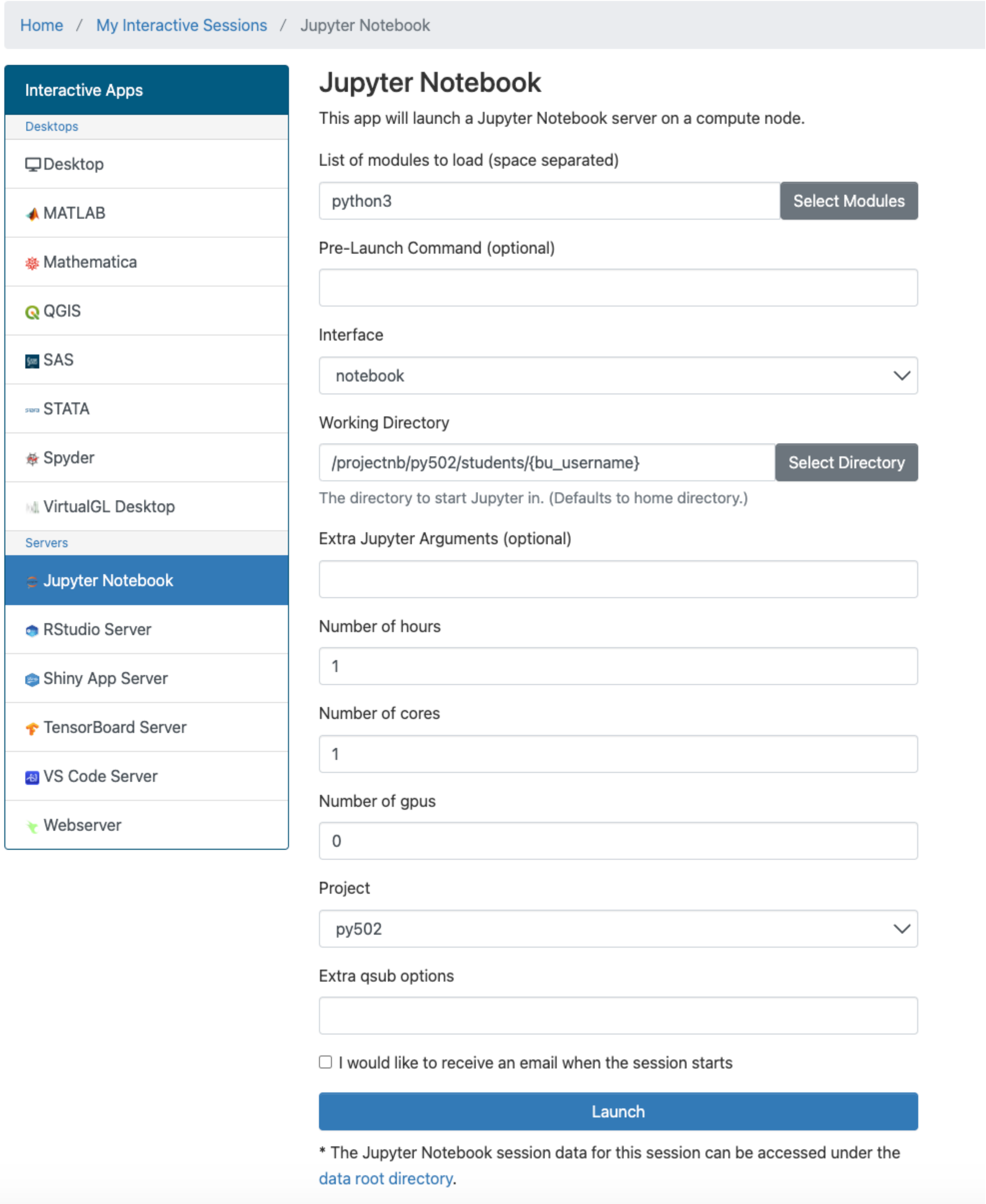
/projectnb/py502/students/{bu_username}

The directory to start Jupyter in. (Defaults to home directory.)



Number of hours

1



Jupyter Notebook

This app will launch a Jupyter Notebook server on a compute node.

List of modules to load (space separated)

python3

Pre-Launch Command (optional)

Interface

notebook

Working Directory

/projectnb/py502/students/{bu_username}

The directory to start Jupyter in. (Defaults to home directory.)

Extra Jupyter Arguments (optional)

Number of hours

1

Number of cores

1

Number of gpus

0

Project

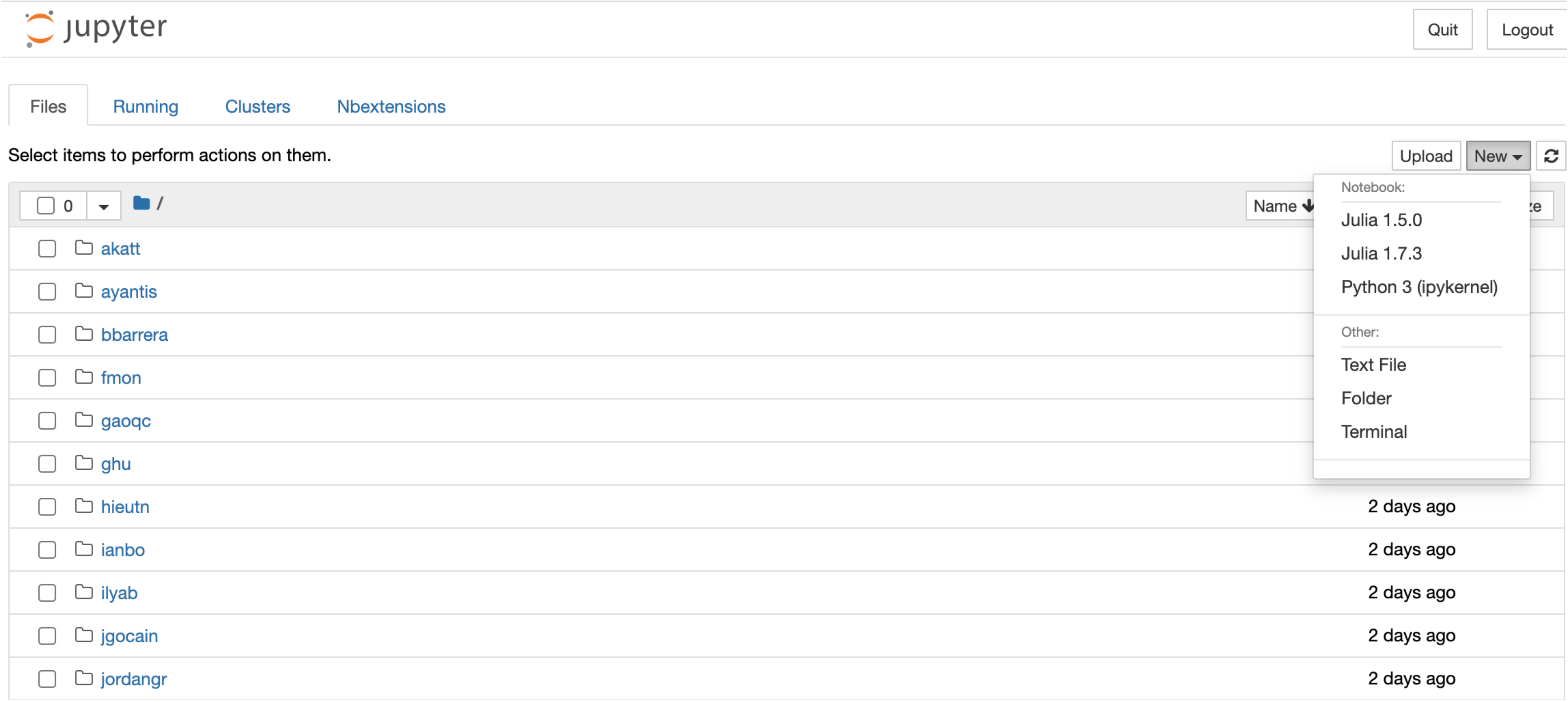
py502

Extra qsub options

☐ I would like to receive an email when the session starts

* The Jupyter Notebook session data for this session can be accessed under the data root directory.

Jupyter Notebook



Select items to perform actions on them.

□ akatt	
□ ayantis	
□ bbarrera	
□ fmon	
□ gaoqc	
□ ghu	
□ hieutn	2 days ago
□ ianbo	2 days ago
□ ilyab	2 days ago
□ jgocain	2 days ago
□ jordangr	2 days ago

Batch Jobs

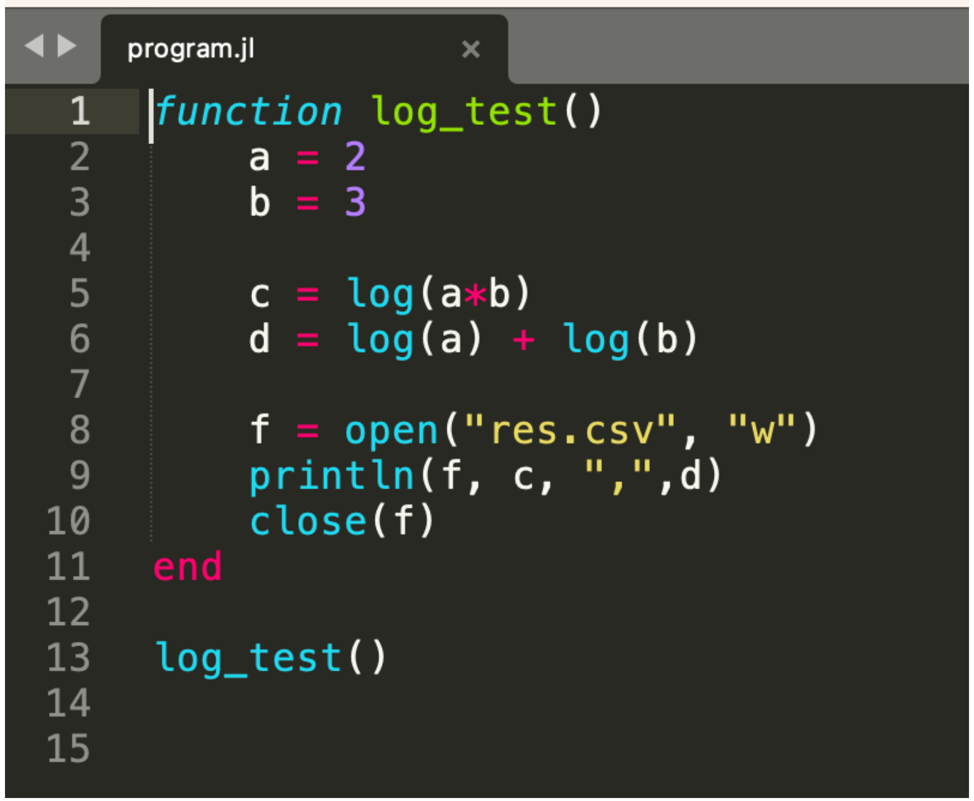
- Submit via terminal using “qsub”
- Run a .jl file (ideally one that runs a function) that outputs data to specified directory
- More info: https://www.bu.edu/tech/support/research/system-usage/running-jobs/submitting-jobs/

Batch Jobs

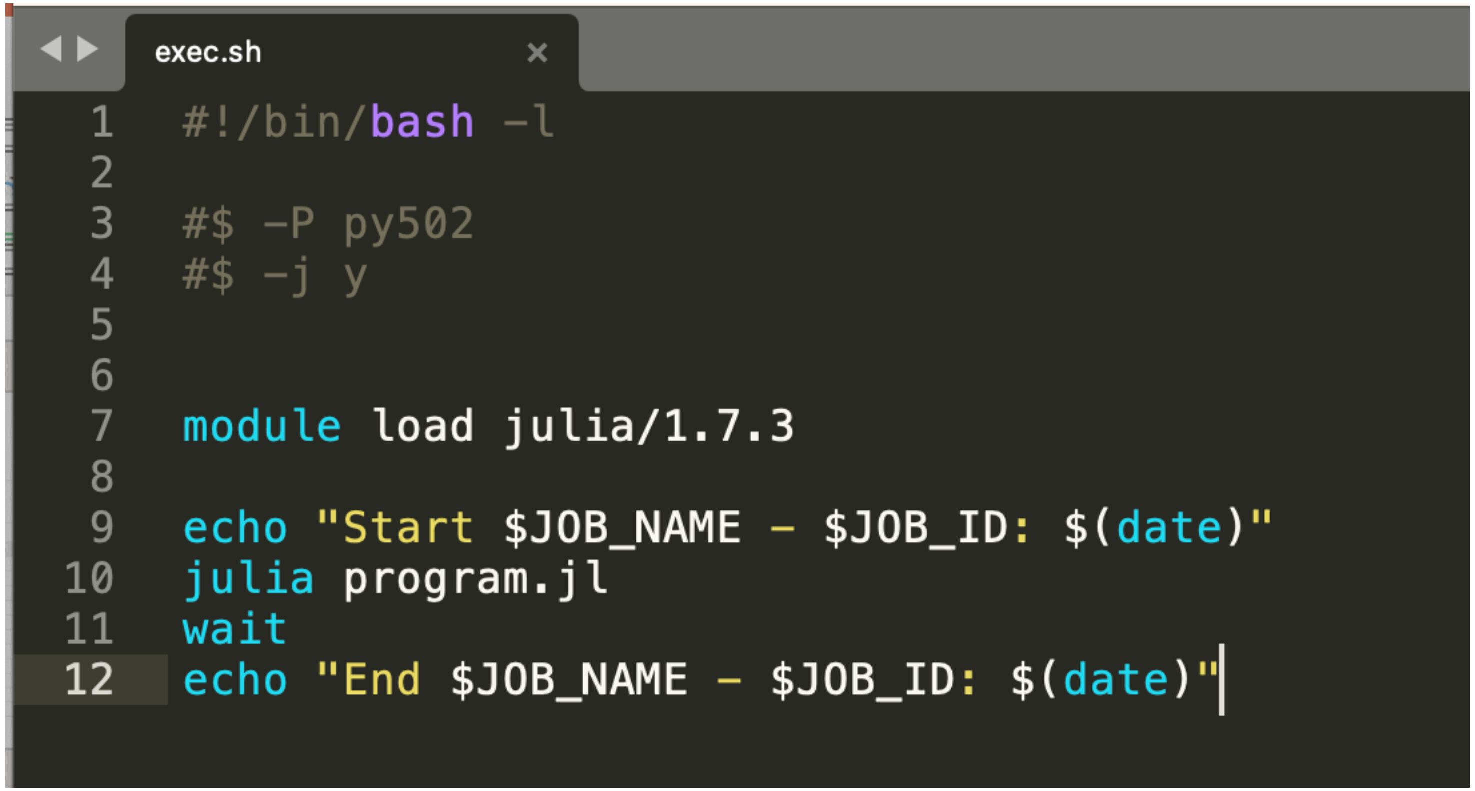
Three pieces of code:

1. Julia code that runs program
   - i.e. .jl file that contains all functions for program with single function call at end
2. Bash script that executes Julia code
   - i.e. `julia run.jl`
3. Bash script that "qsubs" 2 (not strictly necessary)
   - i.e. `qsub exec.sh`

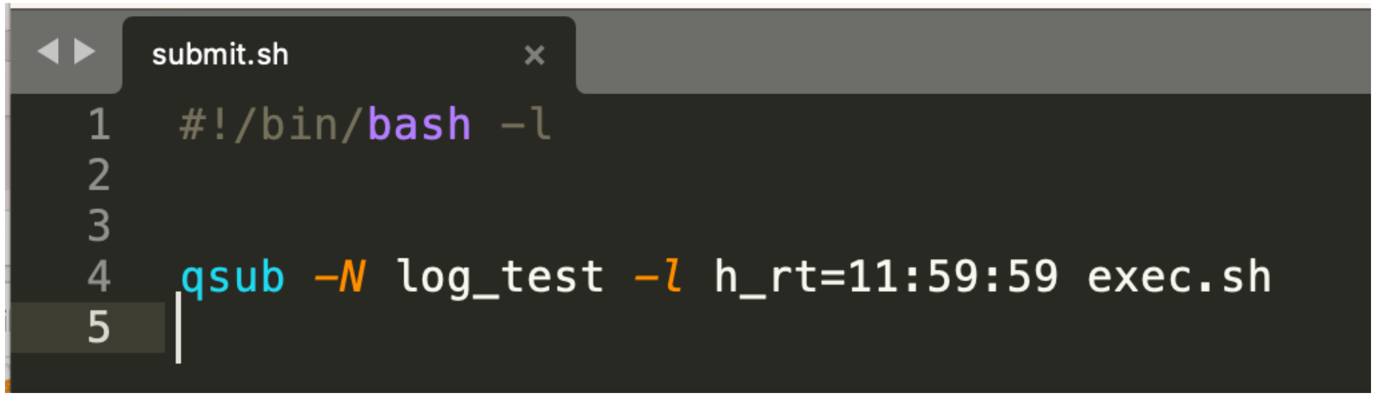
There are various options to specify when using qsub, you can find all the details the RCS website



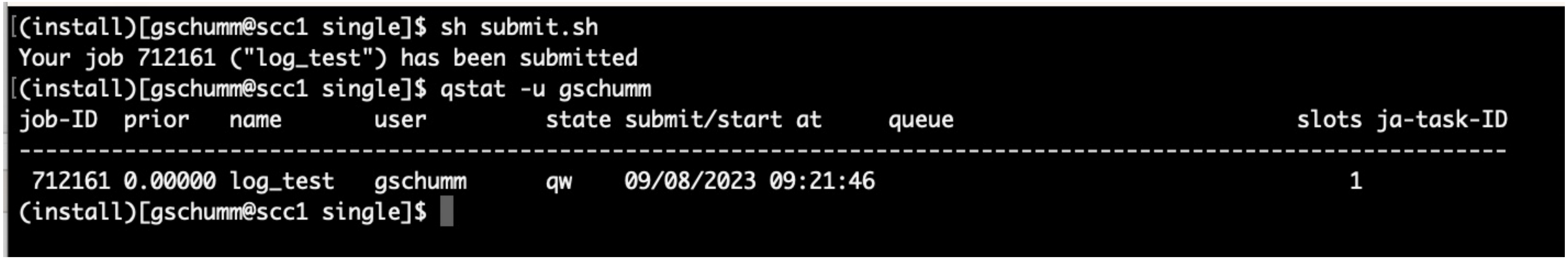
```
function log_test()
    a = 2
    b = 3

    c = log(a*b)
    d = log(a) + log(b)

    f = open("res.csv", "w")
    println(f, c, ",",d)
    close(f)
end

log_test()


```



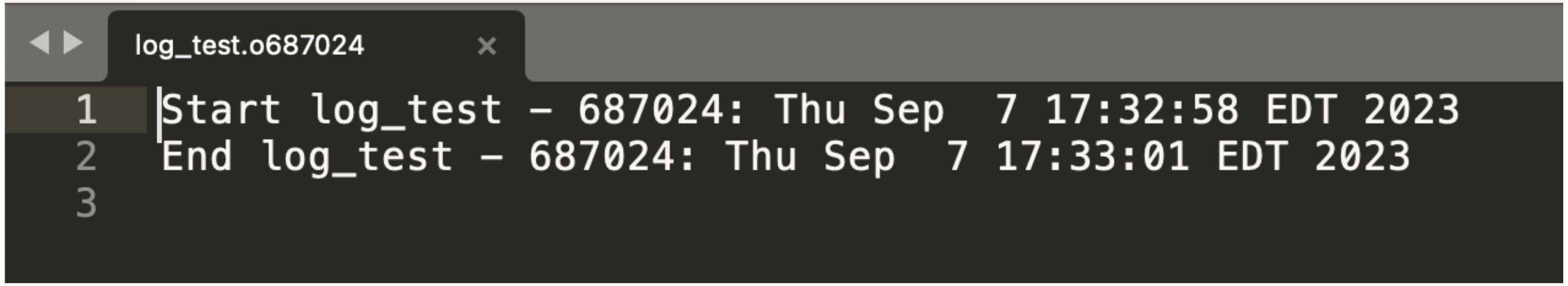
```
#!/bin/bash -l

#$ -P py502
#$ -j y


module load julia/1.7.3

echo "Start $JOB_NAME - $JOB_ID: $(date)"
julia program.jl
wait
echo "End $JOB_NAME - $JOB_ID: $(date)"
```



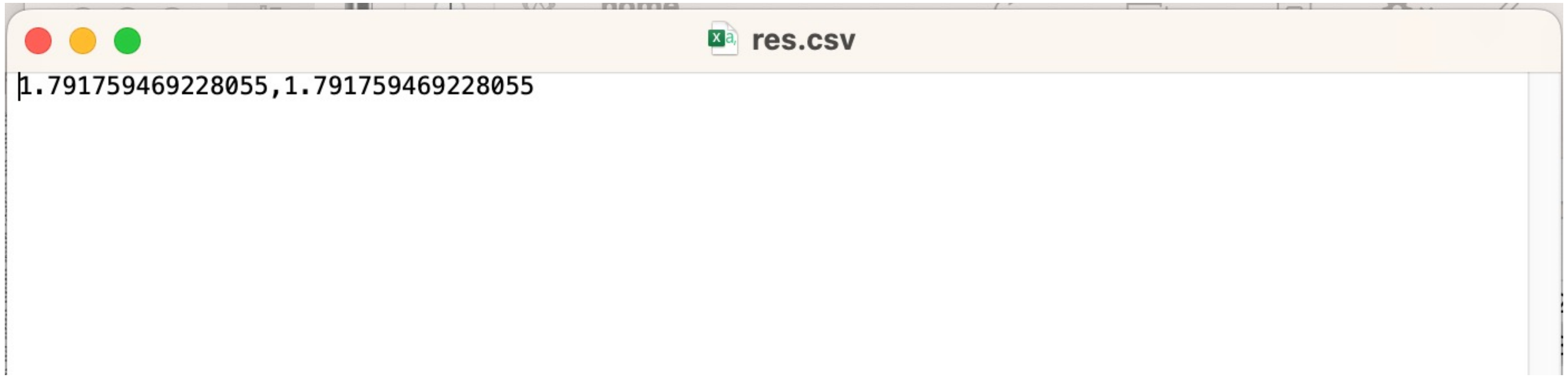
```
#!/bin/bash -l


qsub -N log_test -l h_rt=11:59:59 exec.sh

```



```
(install)[gschumm@scc1 single]$ sh submit.sh
Your job 712161 ("log_test") has been submitted
(install)[gschumm@scc1 single]$ qstat -u gschumm
job-ID  prior   name       user         state submit/start at     queue                          slots ja-task-ID
-----------------------------------------------------------------------------------------------------------------
 712161 0.00000 log_test   gschumm      qw    09/08/2023 09:21:46                                    1
(install)[gschumm@scc1 single]$ 
```



```
Start log_test - 687024: Thu Sep  7 17:32:58 EDT 2023
End log_test - 687024: Thu Sep  7 17:33:01 EDT 2023
```



```
1.791759469228055,1.791759469228055
```