Using BU's Shared Computing Cluster (SCC)

PY502

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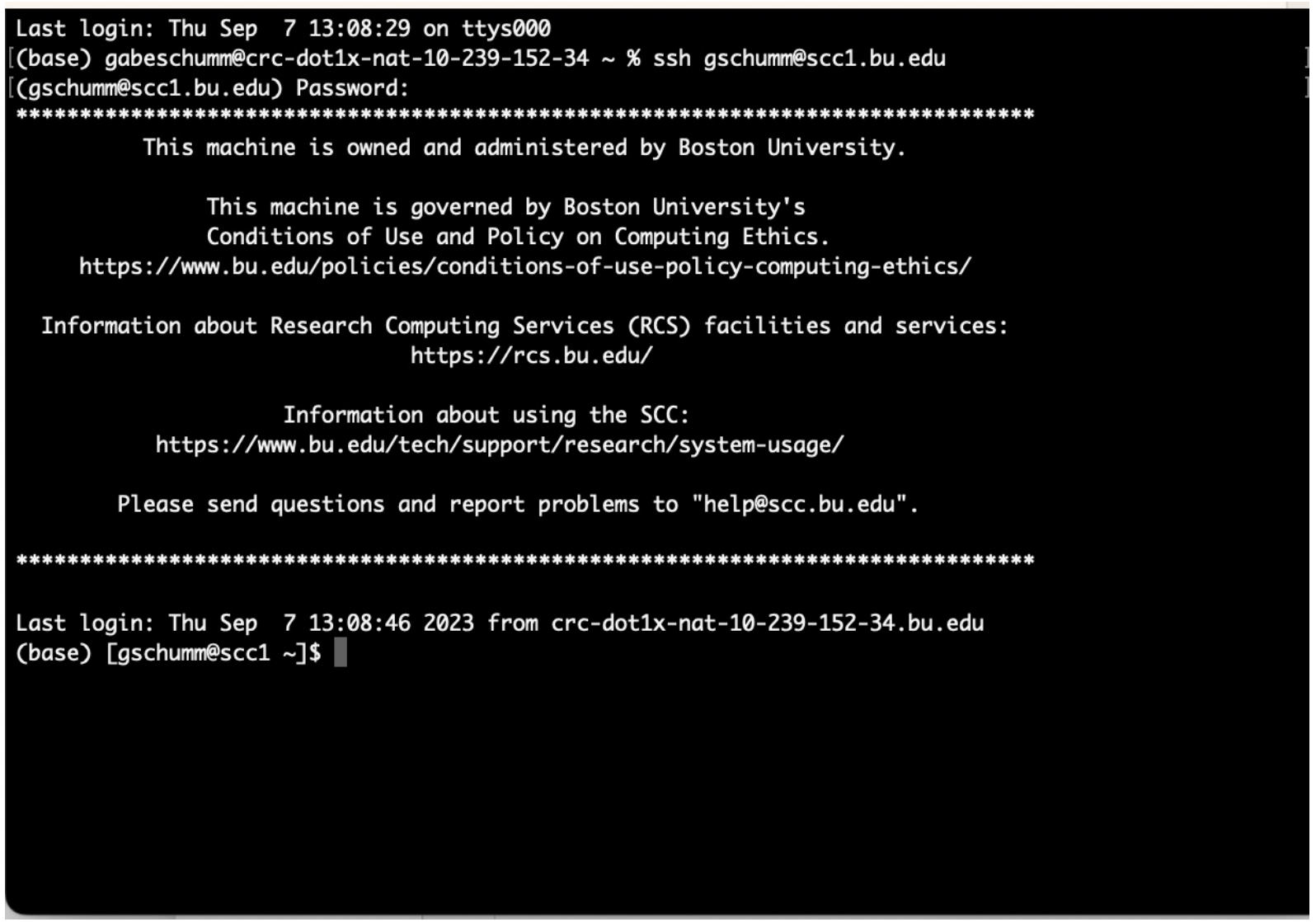
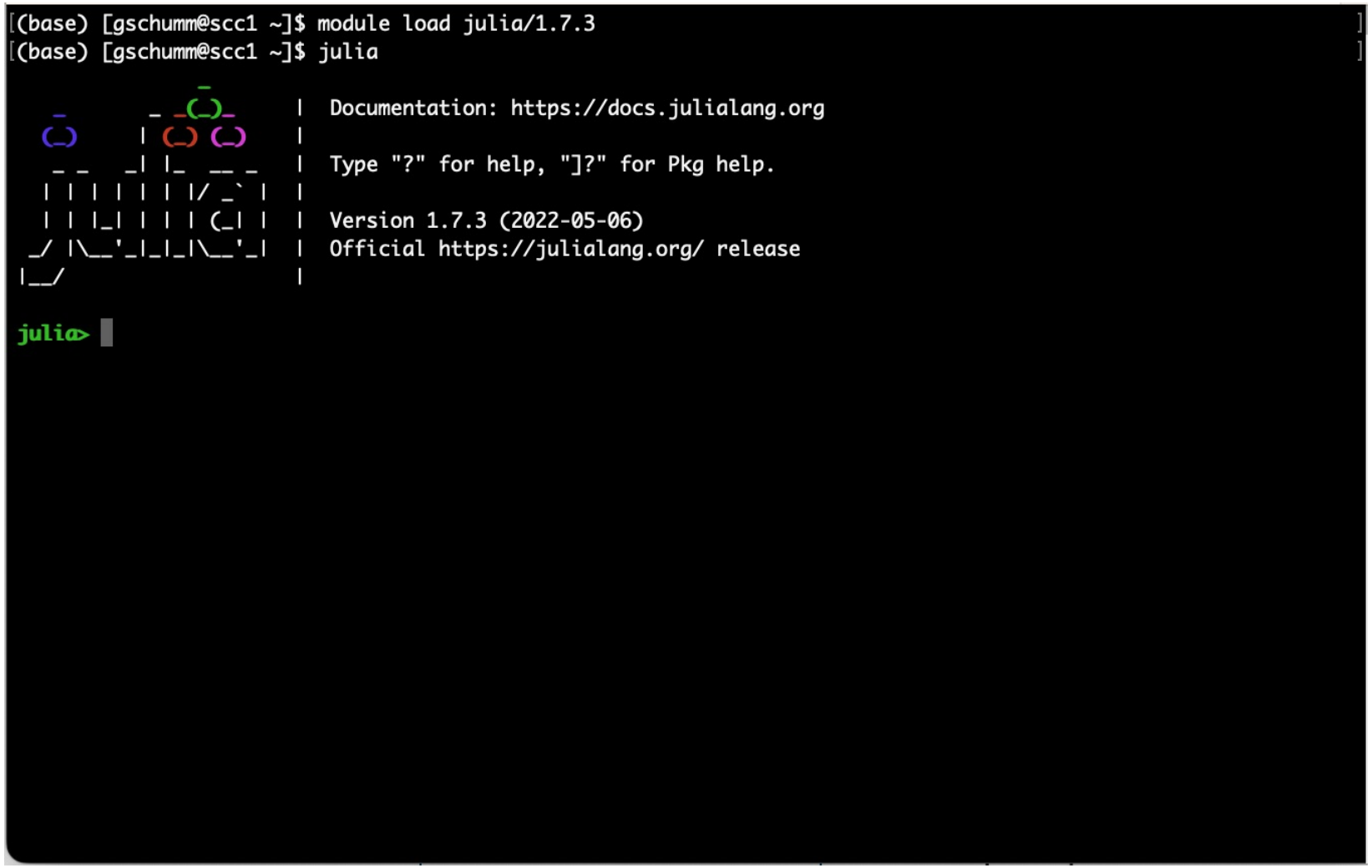
Options

- 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

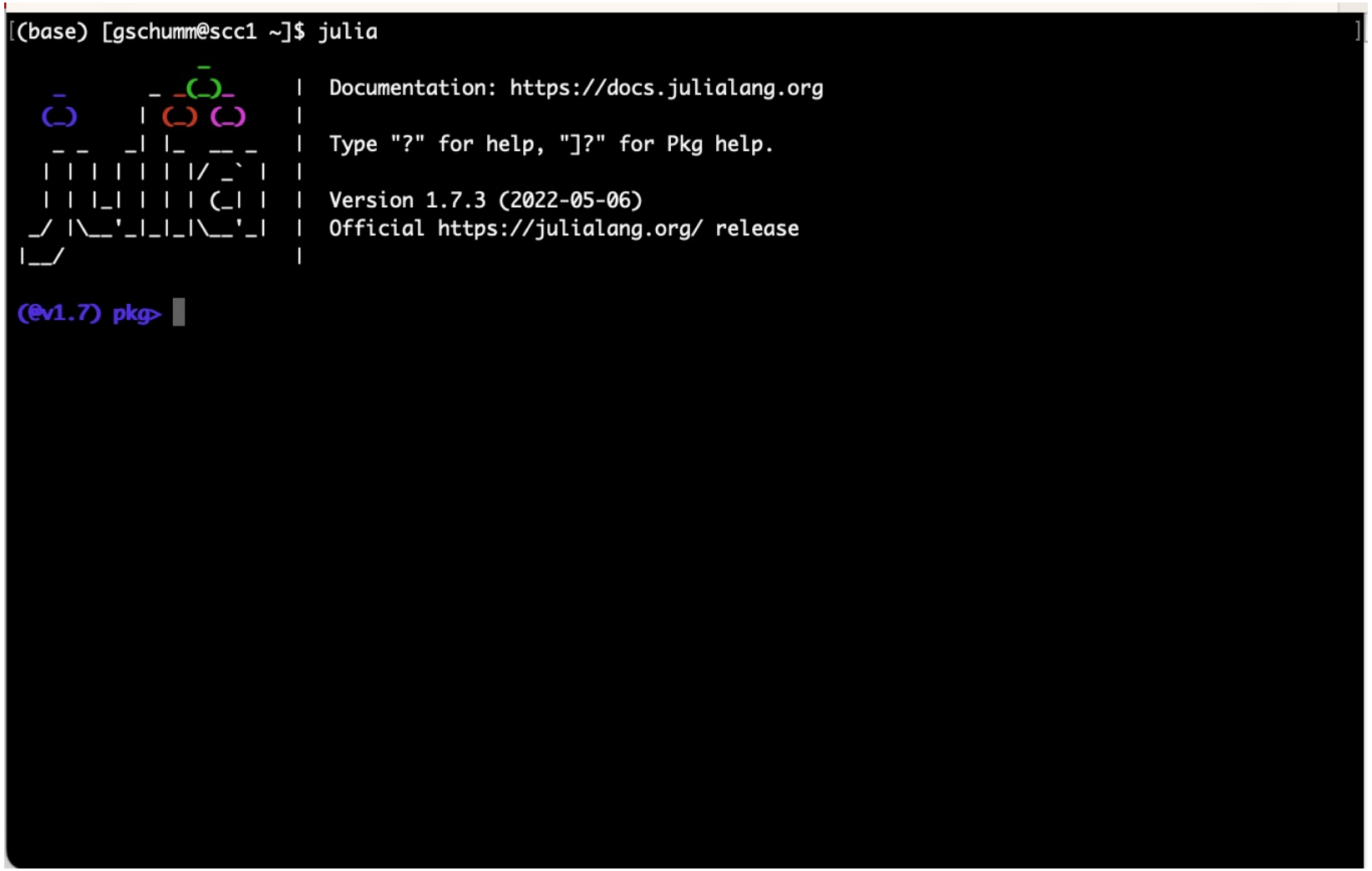


Setting up Julia



Setting up Julia

Type “]” to enter “Pkg REPL”



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

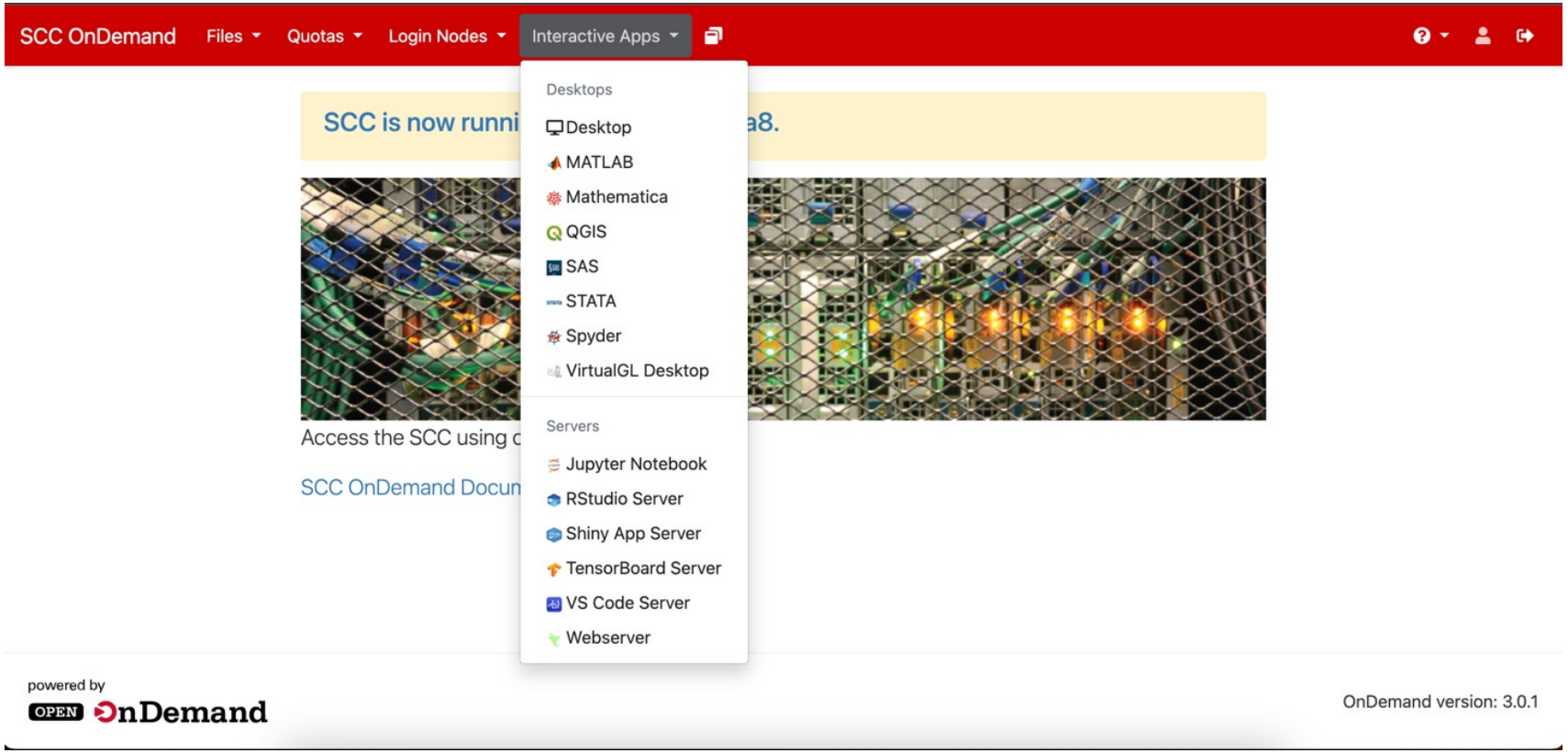
```
(@v1.7) pkg> status
      Status `~/.julia/environments/v1.7/Project.toml`
  [7073ff75] IJulia v1.24.2
  [91a5bcdd] Plots v1.36.6
  [ade2ca70] Dates
  [8bb1440f] DelimitedFiles
  [37e2e46d] LinearAlgebra
  [de0858da] Printf
  [10745b16] Statistics

(@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/



Jupyter Notebook

List of modules to load (space separated)

python3 Select Modules

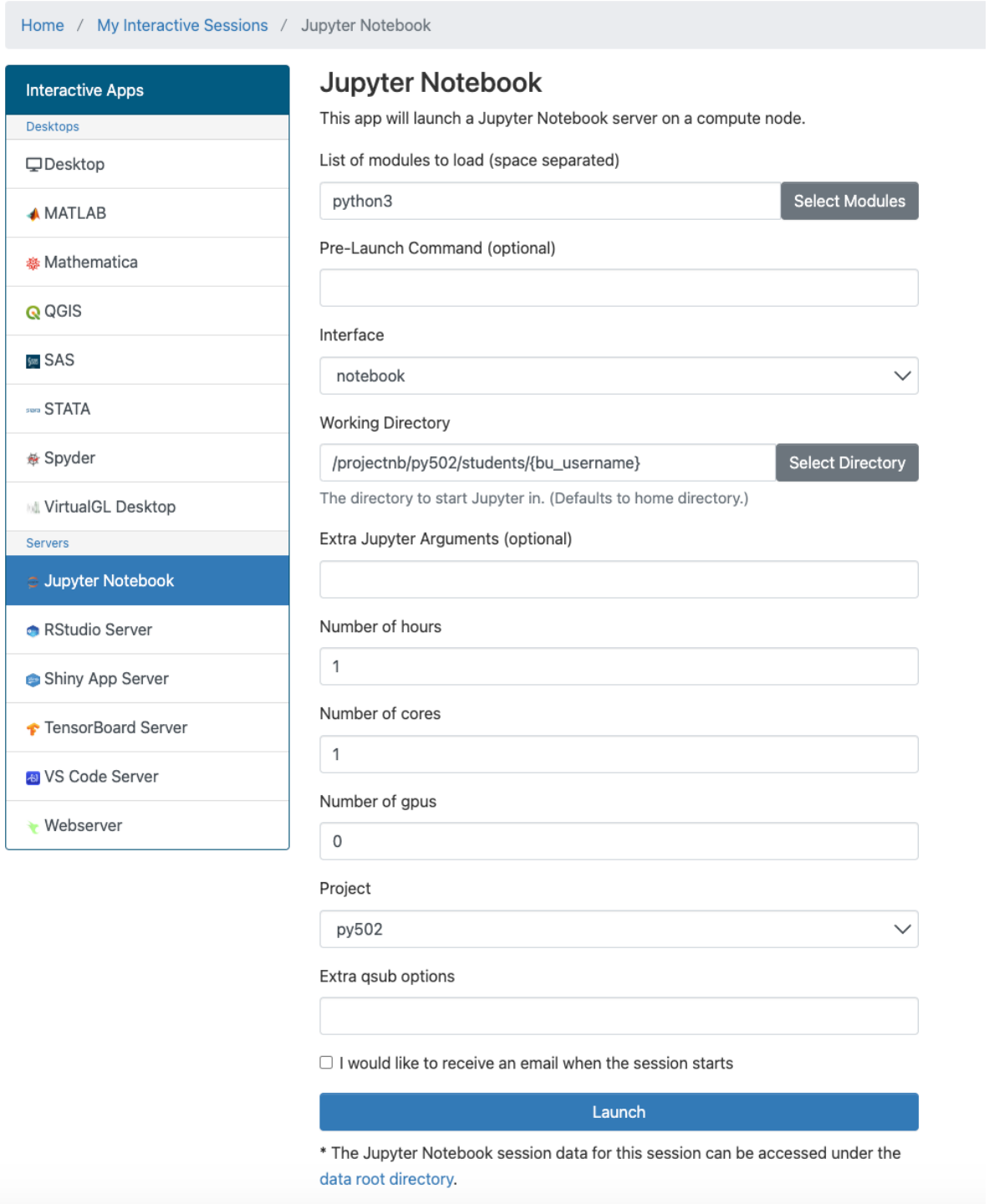
Working Directory

/projectnb/py502/students/{bu_username} Select Directory

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

Number of hours

1



Jupyter Notebook

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

program.jl

```
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()
```

exec.sh

```
#!/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)"
```

submit.sh

```
#!/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]$
```

log_test.o687024

```
1  Start log_test - 687024: Thu Sep  7 17:32:58 EDT 2023
2  End log_test - 687024: Thu Sep  7 17:33:01 EDT 2023
3
```

res.csv

```
1.791759469228055,1.791759469228055
```