

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”
 - **J**upyter 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

```
(@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`

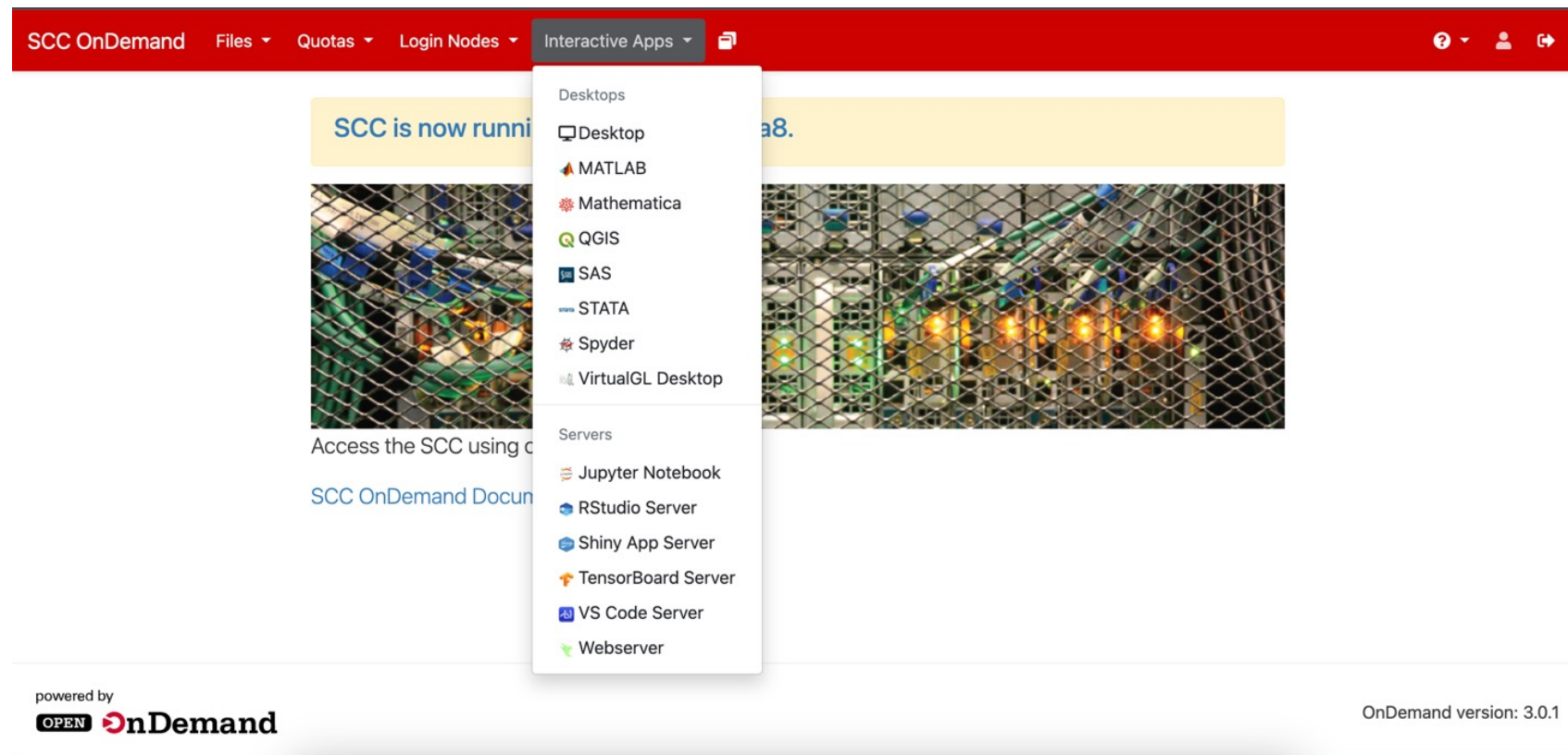
(@v1.7) pkg> █
```

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/>



The screenshot displays the SCC OnDemand web interface. At the top, a red navigation bar contains the text "SCC OnDemand" and several dropdown menus: "Files", "Quotas", "Login Nodes", and "Interactive Apps". The "Interactive Apps" menu is open, showing a list of application categories and specific tools. The background of the page features a yellow banner with the text "SCC is now running on a8." and two images of server racks behind a metal mesh fence. Below the banner, there is a section titled "Access the SCC using c" and a link to "SCC OnDemand Documenta". At the bottom left, the text "powered by" is followed by the "OPEN OnDemand" logo. At the bottom right, the text "OnDemand version: 3.0.1" is displayed.

SCC OnDemand Files Quotas Login Nodes Interactive Apps

SCC is now running on a8.

Access the SCC using c

SCC OnDemand Documenta

powered by OPEN OnDemand

OnDemand version: 3.0.1

Interactive Apps menu items:

- Desktops
 - Desktop
 - MATLAB
 - Mathematica
 - QGIS
 - SAS
 - STATA
 - Spyder
 - VirtualGL Desktop
- Servers
 - Jupyter Notebook
 - RStudio Server
 - Shiny App Server
 - TensorBoard Server
 - VS Code Server
 - Webserver

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

Interactive Apps
Desktops
Desktop
MATLAB
Mathematica
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Spyder
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RStudio Server
Shiny App Server
TensorBoard Server
VS Code Server
Webserver

Jupyter Notebook

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

List of modules to load (space separated)

python3 Select Modules

Pre-Launch Command (optional)

Interface

notebook ▼

Working Directory

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

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

Launch

* The Jupyter Notebook session data for this session can be accessed under the [data root directory](#).

Jupyter Notebook



Quit

Logout

Files

Running

Clusters

Nbextensions

Select items to perform actions on them.

Upload

New ▾



<input type="checkbox"/> 0 ▾	/	Name ▾	
<input type="checkbox"/>	akatt		
<input type="checkbox"/>	ayantis		
<input type="checkbox"/>	bbarrera		
<input type="checkbox"/>	fmon		
<input type="checkbox"/>	gaoqc		
<input type="checkbox"/>	ghu		
<input type="checkbox"/>	hieutn		2 days ago
<input type="checkbox"/>	ianbo		2 days ago
<input type="checkbox"/>	ilyab		2 days ago
<input type="checkbox"/>	jgocain		2 days ago
<input type="checkbox"/>	jordangr		2 days ago

Notebook:

- Julia 1.5.0
- Julia 1.7.3
- Python 3 (ipykernel)

Other:

- Text File
- Folder
- Terminal

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 x
1 function log_test()
2     a = 2
3     b = 3
4
5     c = log(a*b)
6     d = log(a) + log(b)
7
8     f = open("res.csv", "w")
9     println(f, c, ",", d)
10    close(f)
11 end
12
13 log_test()
14
15
```

```
exec.sh x
1 #!/bin/bash -l
2
3 #$ -P py502
4 #$ -j y
5
6
7 module load julia/1.7.3
8
9 echo "Start $JOB_NAME - $JOB_ID: $(date)"
10 julia program.jl
11 wait
12 echo "End $JOB_NAME - $JOB_ID: $(date)"
```

```
submit.sh x
1 #!/bin/bash -l
2
3
4 qsub -N log_test -l h_rt=11:59:59 exec.sh
5
```

```
[(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 x
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
```