INTRODUCTION TO RIVANNA

Last revised: 02/15/2019

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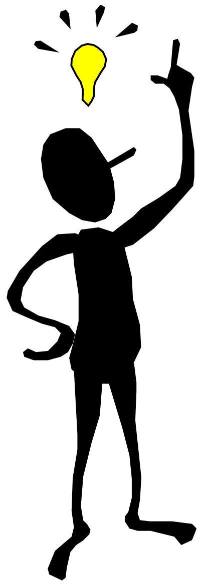
Terminology



- Node
  - Basic building block of a cluster
  - Usually a specialized computer
- Two types of nodes:
  - Head Node – computer used for logging on and submitting jobs
  - Compute Node -- computer that does most of the work
- Core – an individual processor on a computer

ALLOCATIONS & ACCOUNTS

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Allocations

- Rivanna is allocated:

  At the most basic level, an allocation refers to a chunk of CPU time that you receive and can use too run your computation.

- Allocations are measured in service units (SUs), where

  1 SU = 1 core-hour

- All accounts on a given allocation share the service units.

Requesting an Allocation

- Faculty (including postdocs) are eligible for an allocation (see www.arcs.virginia.edu/allocations).
- Students must be sponsored by a PI (e.g., an advisor, a professor, a research mentor).
- The PI must complete the form at
  https://arcs.virginia.edu/allocation
  - To get to the form, scroll down and click on "Request a New or Renewal Standard Allocation"

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CONNECTING & LOGGING ON TO RIVANNA

How to connect to Rivanna

- There are three ways to connect to Rivanna:

1. ssh client
    - Instructions for installing and using an ssh client are provided in the appendix of these slides.

2. FastX
    - Using your web browser, go to URL https://rivanna-desktop.hpc.virginia.edu and log in.
    - Click on "Launch Session"; Select "MATE" and click on "Launch"

3. OpenonDemand https://rivanna-portal.hpc.virginia.edu
    - Authenticates with Netbadge.

Ssh and FastX require the UVa Anywhere VPN when off-grounds.

See http://its.virginia.edu/vpn/ for details.

Connecting to the Cluster

- The hostname for the Interactive frontends:
  rivanna.hpc.virginia.edu

  (does round-robin among the front-ends)

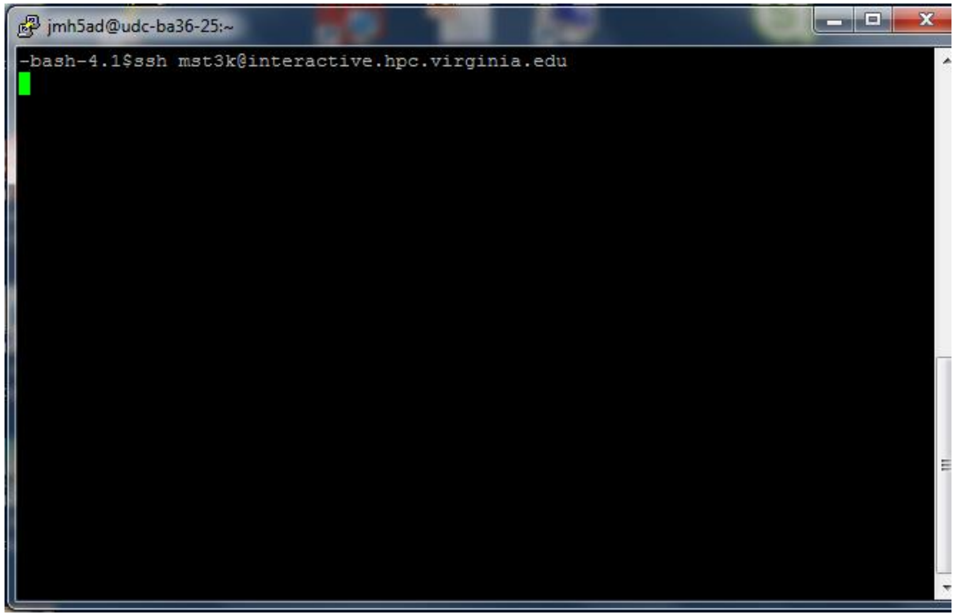
- However, you also can log onto a specific front-end:
  - rivanna1.hpc.virginia.edu
  - rivanna2.hpc.virginia.edu
  - rivanna3.hpc.virginia.edu

Connecting to the Cluster with ssh

- If you are on a Mac or Linux machine your can connect with ssh.
- Bring up a terminal window and type:

  ssh –Y *userID*@rivanna.hpc.virginia.edu

- When it prompts you for for a password, use your Eservices password.


jmh5ad@udc-ba36-25:~

```
-bash-4.1$ssh mst3k@interactive.hpc.virginia.edu
```

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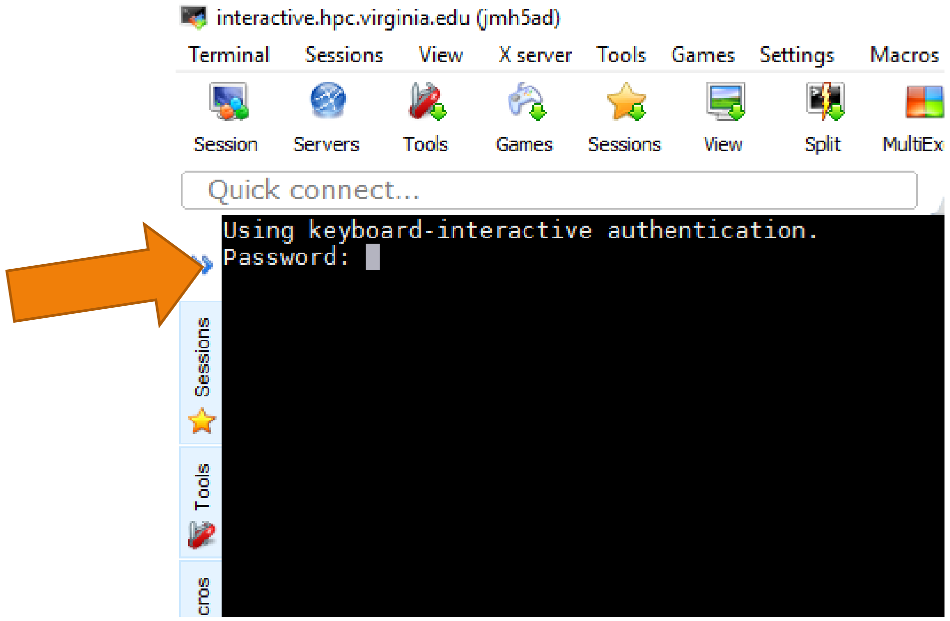
Connecting to the Cluster with MobaXterm

- We recommend MobaXterm for Windows users.
- It will prompt you for your password but will not echo asterisks. It can also remember your password.

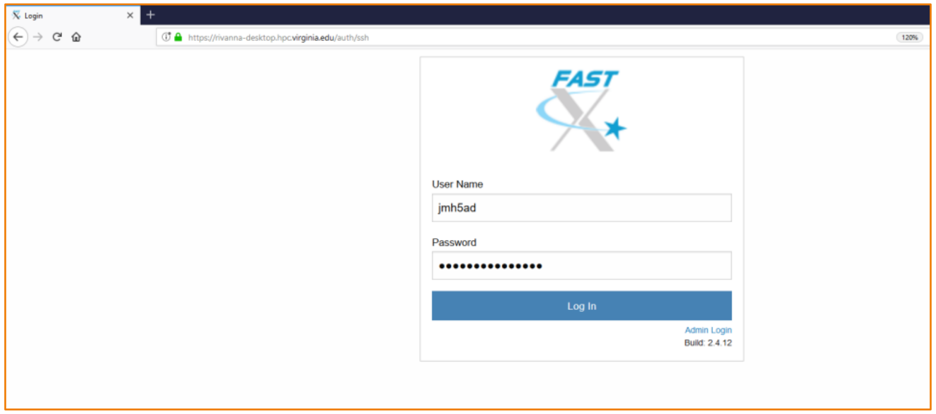

interactive.hpc.virginia.edu (jmh5ad)
Terminal Sessions View X server Tools Games Settings Macros
Session Servers Tools Games Sessions View Split MultiEx
Quick connect...
Sessions
Tools
cros

```
Using keyboard-interactive authentication.
Password:
```

FastX

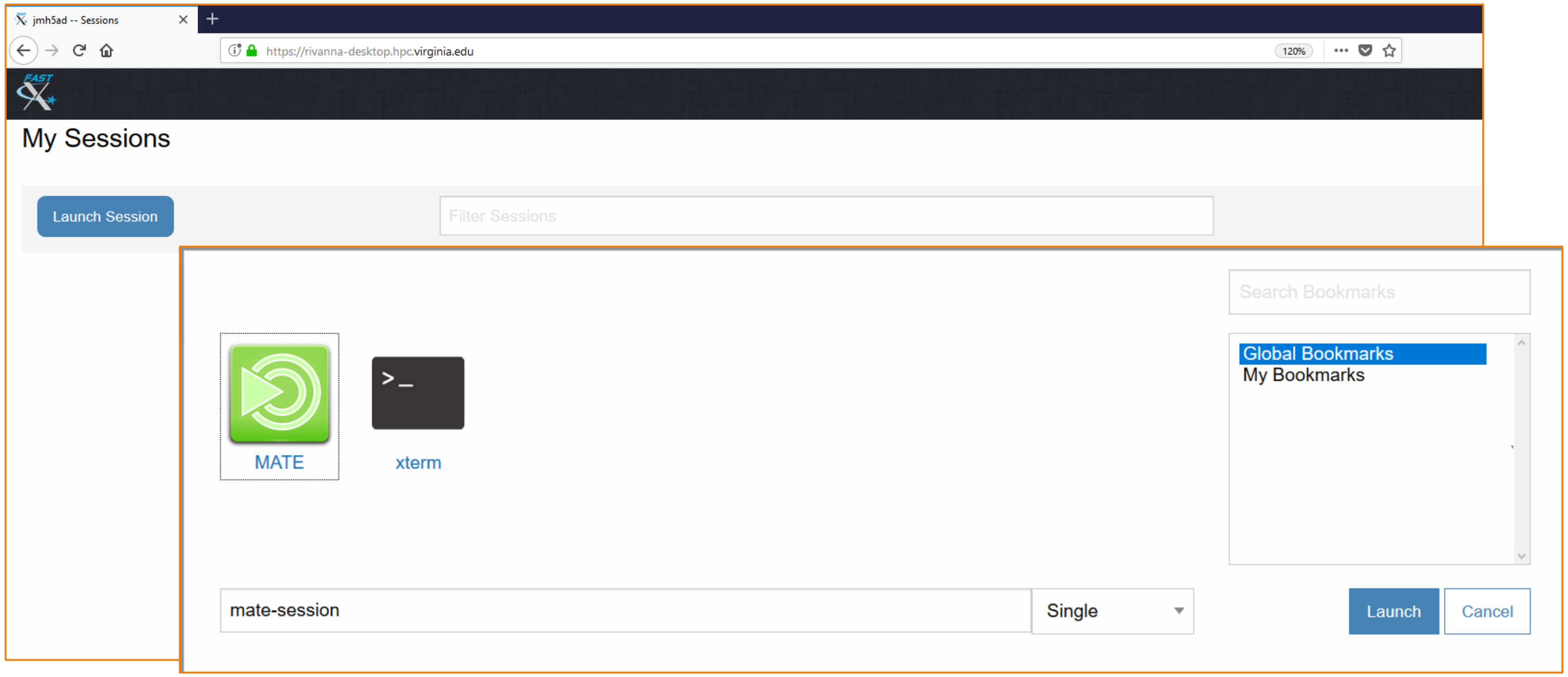
- In your web browser, go to URL:

  https://rivanna-desktop.hpc.virginia.edu



Starting up FastX

- Click "Launch Session"; Select MATE; Click Launch



mate-session

Single

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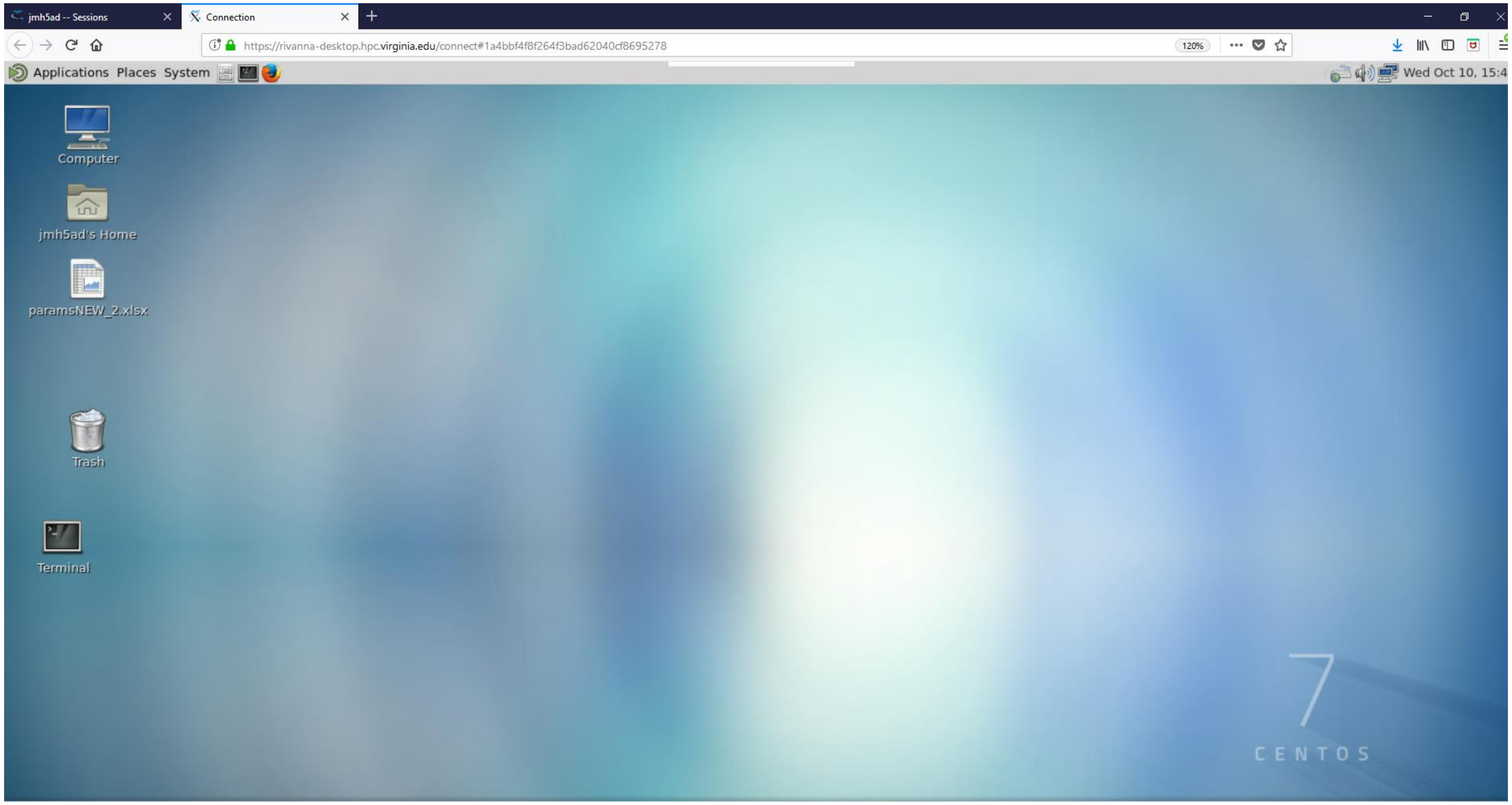
FastX Environment

- A desktop for working on Rivanna


jmh5ad -- Sessions
Connection
https://rivanna-desktop.hpc.virginia.edu/connect#1a4bbf4f8f264f3bad62040cf8695278
120%
Applications Places System
Wed Oct 10, 15:4
Computer
jmh5ad's Home
paramsNEW_2.xlsx
Trash
Terminal
7
CENTOS

CLUSTER ENVIRONMENT

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Your Home Directory

- The default home directory on Rivanna has 50GB of storage capacity
  - This directory is distinct from the 4GB home directory provided by ITS.
  - The ITS home directory is available as `/tiny/$USER`

Checking your Home Storage

- To see how much disk space you have used in your home directory, open a Terminal window and type **`hdquota`** at the command-line prompt:

```
$ hdquota


Filesystem  |  Used  |  Avail  |  Limit  |  Percent Used
  qhome        39G       12G       51G          77%
```

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Leased (Group) Storage

- Groups can lease space for longer-term storage
  - Project: has snapshots.
  - Value: no snapshots
  - Overview at
    - https://arcs.virginia.edu/storage

Your /scratch Directory

- Each user will have access to 10 TB of **temporary** storage.
  - It is located in a subdirectory under /scratch, and named with your userID
  - e.g., `/scratch/mst3k`
  - You are limited to 350,000 files in your scratch directory.

Important:
/scratch is **NOT permanent** storage and files older than **90 days** will be marked for deletion.

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Running Jobs from Scratch

- We recommend that you run your jobs out of your /scratch directory for two reasons:
    - /scratch is on a Lustre filesystem (a storage system designed specifically for parallel access).
    - /scratch is connected to the compute nodes with Infiniband (a very fast network connection).

We also recommend that

- You keep copies of your programs and data in more permanent locations (e.g., your home directory or leased storage).
- After your jobs finish, you copy the results to more permanent storage.

Checking your /scratch Storage

- To see the amount of scratch space that is available to you, type **sfsq** at the command line prompt.

```
$ sfsq

'scratch' usage status for 'mst3k', last
updated: 2016-09-08 16:26:12

 - ~28/10,000 GBs allocated disk space
 - 153/350,000 files created
 - 151/153 files marked for deletion due to
age limits

To view a list of all files marked for
deletion, please run 'sfsq -l'
```

Checking your Allocation

- To see how many SUs you have available for running jobs, type **`allocations`** at the command-line prompt:

```
$ allocations

Allocations available to Misty S. Theatre(mst3k):

 * robot_build: less than 6,917 service-units remaining.
 * gizmonic-testing: less than 5,000 service-units remaining.
 * servo: less than 59,759 service-units remaining, allocation will expire on
2017-01-01.
 * crow-lab: less than 2,978 service-units remaining.
 * gypsy: no service-units remaining
```

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Moving data onto Rivanna

- You have several options for transferring data onto your home or /scratch directories.
  1. Use the scp command in a terminal window.
  2. Use a drag-and-drop option with MobaXterm (Windows) or Fugu (Mac OS). Cyberduck and Filezilla are cross-platform (but always use ssh/scp protocol)
  3. Use OpenOnDemand for small files.
  4. Set up a Globus endpoint on your local computer and use the Globus web interface to transfer files.

     (See https://arcs.virginia.edu/globus for details)

MODULES

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Modules

- Any application software that you want to use will need to be loaded with the `module load` command.
- For example:
    - module load matlab
    - module load anaconda/5.2. 0-py3.6
    - module load gcc R/3.5.1
- You will need to load the module any time that you create a new shell
    - Every time that you log out and back in
    - Every time that you run a batch job on a compute node

Module Details

- `module avail` – Lists all available modules and versions for a given hierarchy (compiler or compiler+MPI).
- `module spider` – Shows all available modules
- `module key <keyword>` – Shows modules with the keyword in the description
- `module list` – Lists modules loaded in your environment.
- `module load mymod` – Loads the default module to set up the environment for some software.
  - module load mymod/N.M – Loads a specific version
- `module purge` – Clears all modules.

Learning more about a Module

- To locate a python module, try the following:

```
  $ module avail python

  $ module spider python

  $ module key python
```

- To find chemistry/materials software packages, try this:

```
  $ module key chem
```

- The available software is also listed on our website:
  https://arcs.virginia.edu/software-list

PARTITIONS (QUEUES)

Partitions (Queues)

- Rivanna has several partitions (or queues) for job submissions.
  - You will need to specify a partition when you submit a job.
  - To see the partitions that are available to you, type `queues` at the command-line prompt.

```
$ queues

Queue        Availability   Time       Queue    Maximum    Maximum    Idle    SU     Usable
(partition)  (idle%)        Limit      Limit    Cores/Job  Mem/Core   Nodes   Rate   Accounts

standard     43 13(72.2%)   7-days     none     20         64-GB      195     1.00   robot-build, gypsy
dev          1833(65.2%)    1 hours    none     4          254GB      59      0.00   robot-build, gypsy
parallel     3528(73.5%)    3-days     none     240        64-GB      176     1.00   robot-build, gypsy
largemem     48(60.0%)      7-days     none     16         500-GB     3       1.00   robot-build, gypsy
gpu          334(85.0%)     3-days     none     8          128-GB     10      1.00   robot-build, gypsy
knl          2048(100.0%)   3-days     none     2048       1-GB       8       1.00   robot-build, gypsy
```

Compute Node Partitions (aka Queues)

Queue Name	Purpose	Job Time Limit	Memory / Node	Cores / Node	# of Available Nodes	SU / Core Hour
standard	For jobs on a single compute node	7 days	256 GB 384 GB	28 40	26+108	1.0
gpu	For jobs that can use general purpose graphical processing units (GPGPUs) (K80 or P100)	3 days	256 GB	28	13 (max 4 nodes per job)	1.0 (may go up to 2.0)
parallel	For large parallel jobs on up to 120 nodes (<= 2400 CPU cores)	3 days	128 GB	20	220 (shared w/ standard queue)	1.0
largemem	For memory intensive jobs (<= 16 cores/node)	7 days	1 TB	16	5 (max 2 per user)	1.0
dev	To run jobs that are quick tests of code	1 hour	128 GB	4	2	0.0

SLURM SCRIPTS

SLURM

- SLURM is the Simple Linux Utility for Resource Management.
  - It manages the hardware resources on the cluster (e.g. compute nodes/cpu cores, compute memory, etc.).
- SLURM allows you to request resources within the cluster to run your code.
  - It is used for submitting jobs to compute nodes from an access point (generally called a *frontend*).
  - Frontends are intended for editing, compiling, and very short test runs.
  - Production jobs go to the compute nodes through the resources manager.
- SLURM documentation:

  https://arcs.virginia.edu/slurm

  http://slurm.schedmd.com/documentation.html

SLURM Script

- A SLURM script is a bash script with SLURM directives (#SBATCH) and command-line instructions for running your program.

```
#!/bin/bash
#SBATCH --nodes=1                #total number of nodes for the job
#SBATCH --ntasks=1               #how many copies of code to run
#SBATCH --time=1-12:00:00        #amount of time for the whole job
#SBATCH --partition=standard     #the queue/partition to run on
#SBATCH --account=myGroupName    #the account/allocation to use

module purge
module load gcc/7.1.0            #load modules that my job needs
./mycode                         #command-line execution of my job
```

Submitting a SLURM Job

- To submit the SLURM command file to the queue, use the **`sbatch`** command at the command line prompt.

- For example, if the script on the previous slide is in a file named job_script.slurm, we can submit it as follows:

```
-bash-4.1$ sbatch job_script.slurm
Submitted batch job 18316
```

Checking Job Status

- To display the status of only your ***active*** jobs, type:

  `squeue –u <your_user_id>`

```
-bash-4.1$ squeue –u mst3k

JOBID    PARTITION    NAME      USER    ST    TIME    NODES   NODELIST(REASON)
18316    standard     job_sci   mst3k   R     1:45     1      udc-aw38-34-1
```

- The `squeue` command will show pending jobs and running jobs, but not failed, canceled or completed job.

Checking Job Status

- To display the status of all jobs, type:

  sacct -S <start_date>

```
-bash-4.1$ sacct -S 2019-01-29

3104009       RAxML_NoC+   standard  hpc_build          20   COMPLETED       0:0
3104009.bat+       batch             hpc_build          20   COMPLETED       0:0
3104009.0     raxmlHPC-+             hpc_build          20   COMPLETED       0:0
3108537       sys/dashb+        gpu  hpc_build           1  CANCELLED+       0:0
3108537.bat+       batch             hpc_build           1   CANCELLED      0:15
3108562       sys/dashb+        gpu  hpc_build           1     TIMEOUT       0:0
3108562.bat+       batch             hpc_build           1   CANCELLED      0:15
3109392       sys/dashb+        gpu  hpc_build           1     TIMEOUT       0:0
3109392.bat+       batch             hpc_build           1   CANCELLED      0:15
3112064             srun        gpu  hpc_build           1      FAILED       1:0
3112064.0           bash             hpc_build           1      FAILED       1:0
```

- The `sacct` command lists all jobs (pending, running, completed, canceled, failed, etc.) since the specified date.

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Deleting a Job

- To delete a job from the queue, use the **scancel** command with the job ID number at the command line prompt:

```
-bash-4.1$ scancel 18316
```

MORE ADVANCED JOBS

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High Throughput Job

- High throughput computing (HTC) runs a large number of serial jobs (or sometimes minimally parallel jobs).
- Usually the computations are identical but may use different input files and should produce different output files.
- Job arrays are usually the best way to handle HTC.
- You also can use job arrays to organize the input and output.

Job Arrays

- Create a batch script describing how to do *one* job.

```
#!/bin/bash
#SBATCH --nodes=1                  #total number of nodes for the job
#SBATCH --ntasks=1                 #how many processes I will run
#SBATCH --time=00:05:00            #amount of time for the whole job
#SBATCH --partition=standard       #the queue/partition I will run on
#SBATCH --account=Your_group_name #the account/allocation

module purge
module load gcc R/3.4.0
#command-line execution of my job with command-line arguments

Rscript hello.R ${SLURM_ARRAY_TASK_ID} `pwd`
```

- And, submit by typing:

```
sbatch --array=1-30 hello.slurm
```

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Job Array Numbering

- An increment can be provided

```
sbatch --array=1-7:2 myjob.sh
```

  - This will number them 1, 3, 5, 7

- Or provide a list

```
sbatch --array=1,3,4,5,7,9 myjobs.sh
```

Job Array Environment Variables

- Each job will be provided an environment variable

  `SLURM_ARRAY_JOB_ID`

- And each task will be assigned

  `SLURM_ARRAY_TASK_ID`

  based on the numbers in the range or list specified with --array.

- You can use these environment variables as labels for input/output files, directories, etc.
  - In the SLURM script, a variable

    `%A` represents the overall `SLURM_ARRAY_JOB_ID` and
    `%a` represents `SLURM_ARRAY_TASK_ID`

  - These variables can be used with output and input file names.

Array Script

- Job arrays *should* be named (most jobs don't have to be named).

```
#SBATCH --job-name=<name>
```

or

```
#SBATCH -J <name>
```

- All subjobs will use the same global resource requests.

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Output File Specifications

- It would be prudent to separate stdout and stderror in this case, and give them names corresponding to job and task IDs, such as:

```
#SBATCH -o myjobs.%A_%a.out
#SBATCH -e myjobs.%A_%a.err
```

Hands-on Activity:

Modify the file 02_jobArray/hello.slurm to create separate files for output and error.

Multicore in SLURM

- Multicore programs run on a single node
- Different libraries, example will be for OpenMP
- SLURM scripts for multicore programs should use the following combination of directives:

```
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=M
#where M is replaced
#with the actual number
#of cores that you want
```

Requesting Cores for Threads

- Update SLURM script

```
pluma hello_mc.slurm
```

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=10      #number of cores requested
#SBATCH --time=00:10:00
#SBATCH --partition=standard
#SBATCH --account=<Your_group_name>

module purge
module load gcc
export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}
./myexec
```

- And, submit by typing:

```
sbatch hello_mc.slurm
```

Multinode in SLURM

- Multinode programs run across nodes. Nearly all use MPI.
- SLURM scripts for multinode programs should use the following combination of directives:

```
#SBATCH --nodes=N
#SBATCH --ntasks-per-node=M
#SBATCH --partition=parallel
```

- Try to fill nodes when possible (20 cores per node on parallel)

Requesting Cores for MPI

```
#!/bin/bash
#SBATCH --nodes=5
#SBATCH –ntasks-per-node=20
#SBATCH --time=00:10:00
#SBATCH --partition=parallel
#SBATCH --account=<Your_group_name>

module purge
module load intel
module load intelmpi
srun myexec
```

- And, submit by typing:

```
sbatch hello_mc.slurm
```

ACCESSING GPU NODES

Using GPUs

- Certain applications can utilize for general purpose graphics processing units (GPGPUs) to accelerate computations.
- GPGPUs on Rivanna:
  - K80: dual GPUs per board, can do double precision
  - P100: single GPUs per board, double precision is software (slow), better for machine learning
  - More on the way (1 V100, 2 RTX2080)
  - Build with gcc/5.4.0
- You must first request the `gpu` queue. Then with the `gres` option, type the architecture (if you care) and the number of GPUs.

```
#SBATCH -p gpu
#SBATCH --gres=gpu:k80:2
```

JupyterLab

- JupyterLab is a web-based tool that allows multiple users to run Jupyter notebooks on a remote system.

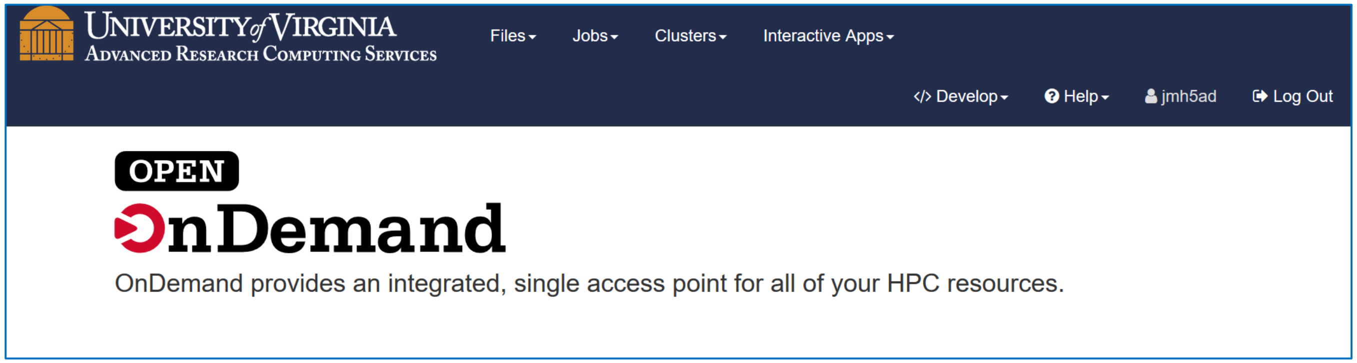
- We now provide JupyterLab on Rivanna.

Accessing JupyterLab

- To access JupyterLab, type the following in your web browser:

  https://rivanna-portal.hpc.virginia.edu/

- After logging in via Netbadge in, you will be directed to the Open OnDemand main page.



OnDemand provides an integrated, single access point for all of your HPC resources.

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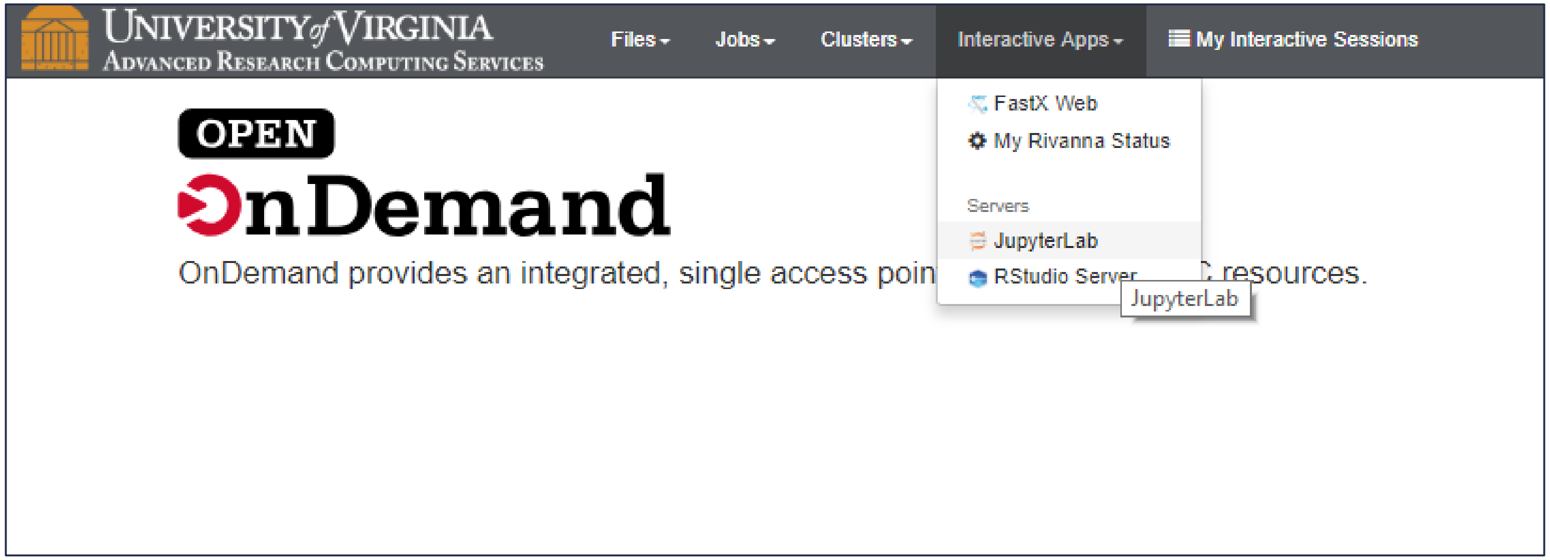
Starting Jupyter Instance

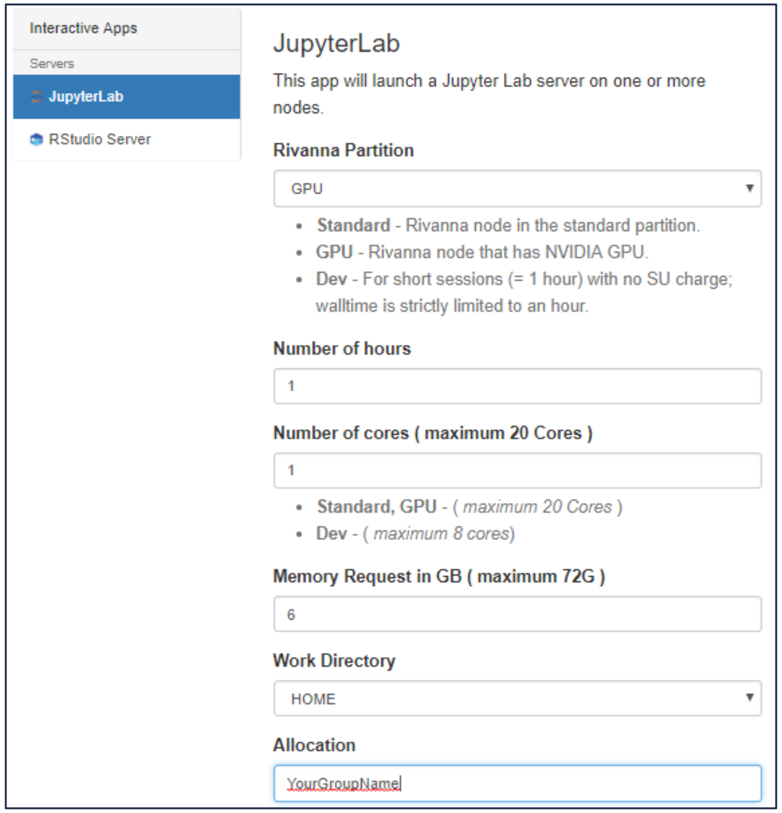
- In the top, click on “Interactive Apps” and in the drop-down box, click on “Jupyter Lab”.



OnDemand provides an integrated, single access poin… resources.

Starting a Jupyter Instance

- A form will appear that allows you to specify the resources for your Notebook.
  - Our example will be using TensorFlow; so, we need to make sure that we select the Rivanna Partition called "GPU".
  - Also, don't forget to put in your "MyGroup" name for the Allocation
  - Finally, click the blue "Launch" button at the bottom of the form (not shown here).



JupyterLab

This app will launch a Jupyter Lab server on one or more nodes.

Rivanna Partition

GPU

- **Standard** - Rivanna node in the standard partition.
- **GPU** - Rivanna node that has NVIDIA GPU.
- **Dev** - For short sessions (= 1 hour) with no SU charge; walltime is strictly limited to an hour.

Number of hours

1

Number of cores (maximum 20 Cores)

1

- **Standard, GPU** - (*maximum 20 Cores*)
- **Dev** - (*maximum 8 cores*)

Memory Request in GB (maximum 72G)

6

Work Directory

HOME

Allocation

YourGroupName

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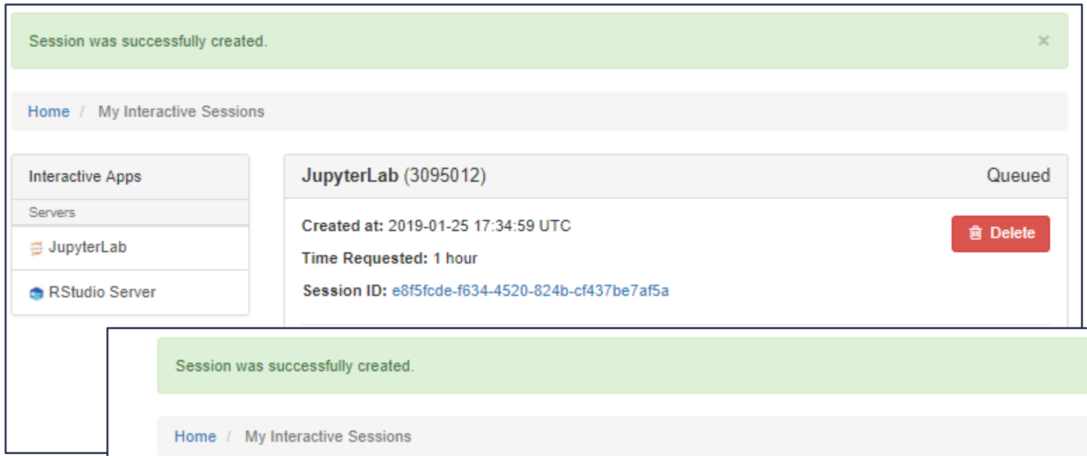
Starting a Jupyter Instance

- It may take a little bit of time for the resources to be allocated.



Session was successfully created.

Home / My Interactive Sessions

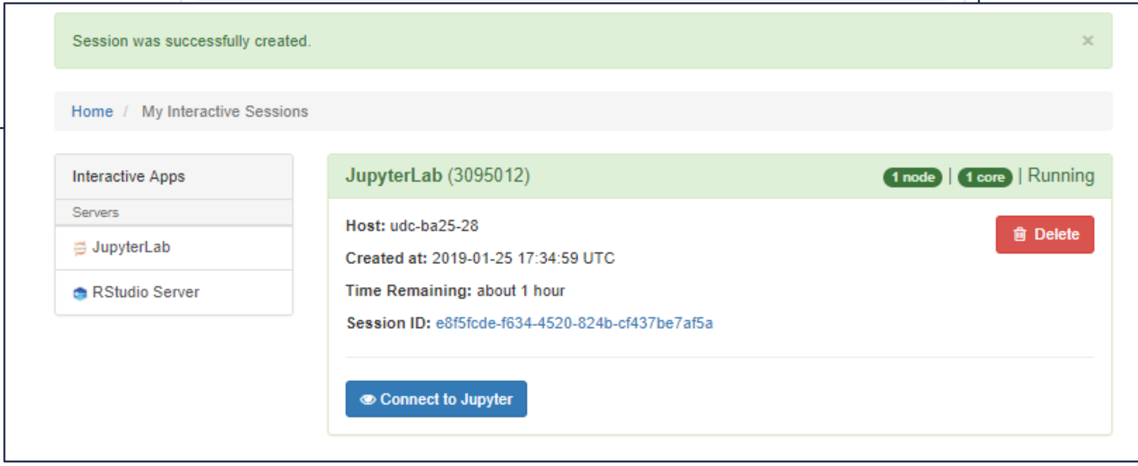
Interactive Apps
Servers
JupyterLab
RStudio Server

JupyterLab (3095012) Queued

Delete

Created at: 2019-01-25 17:34:59 UTC
Time Requested: 1 hour
Session ID: e8f5fcde-f634-4520-824b-cf437be7af5a

- Wait until a blue button with "Connect to Jupyter" appears.



Session was successfully created.

Home / My Interactive Sessions

Interactive Apps
Servers
JupyterLab
RStudio Server

JupyterLab (3095012) 1 node | 1 core | Running

Delete

Host: udc-ba25-28
Created at: 2019-01-25 17:34:59 UTC
Time Remaining: about 1 hour
Session ID: e8f5fcde-f634-4520-824b-cf437be7af5a

Connect to Jupyter

- Click on the blue button.

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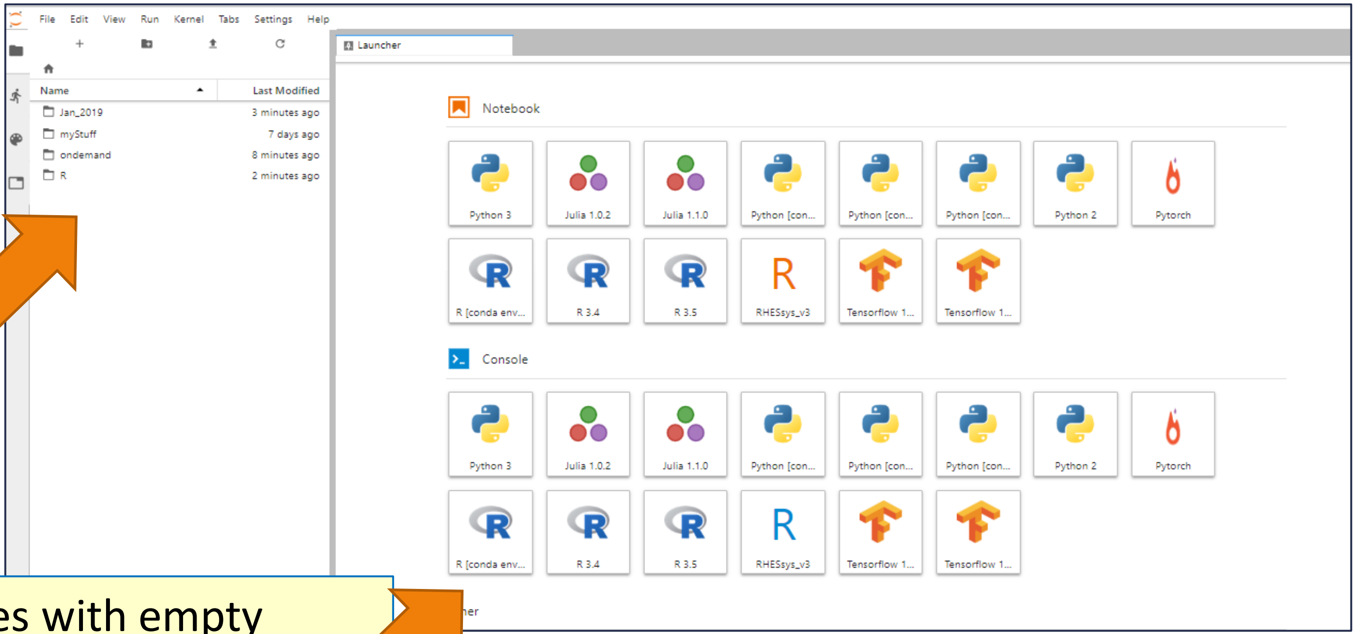
JupyterLab Environment

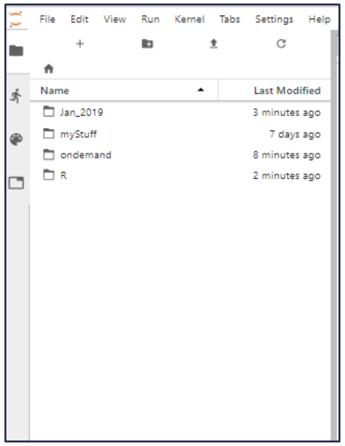


You should see a list of folders and files in your home directory.

And, a set of tiles with empty notebooks or consoles.

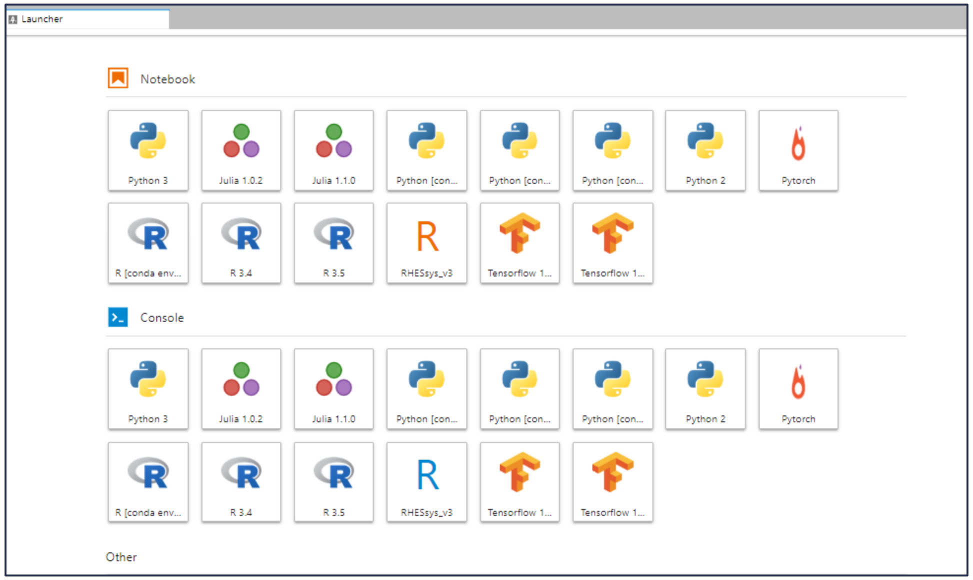
Opening a Notebook

- If you have an existing notebook, you can use the left-pane to maneuver to the file and click on it to open it.



Name	Last Modified
Jan_2019	3 minutes ago
myStuff	7 days ago
ondemand	8 minutes ago
R	2 minutes ago

- Or, if you want to start a new notebook, you can click on the notebook tile, for the appropriate underlying system.



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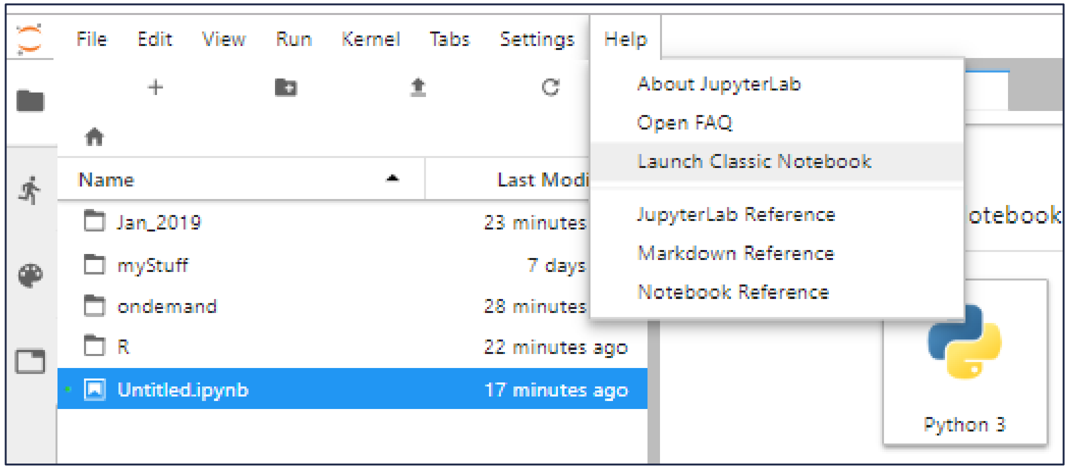
Classic Notebook

- If you feel more comfortable working with the former Jupyter interface, you can select:

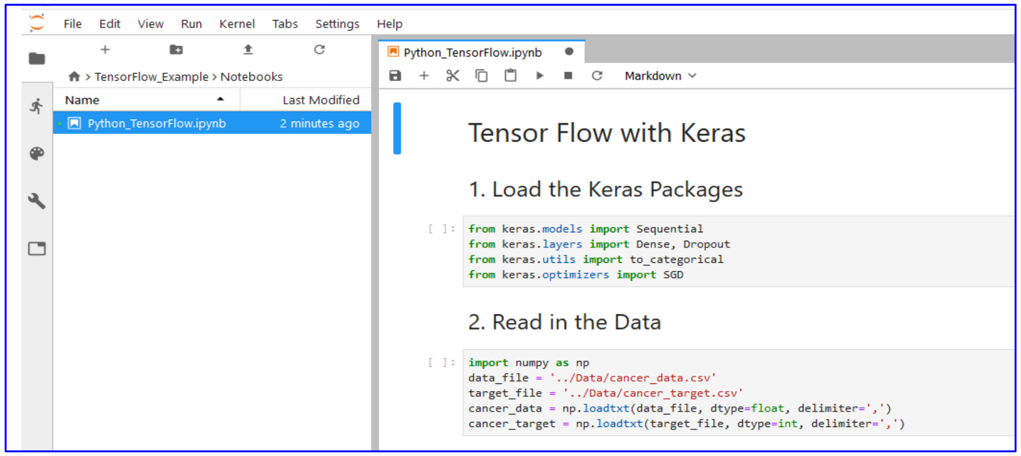
  Help> Launch Classic Notebook



- But, for our example, we will stay with the Jupyter Lab format.

Cautions

- Any changes that you make to the notebook may be saved automatically.
- When the time for your session expires, the session will end without warning.
- Your Jupyter session will continue running until you delete it.
  - Go back to the "Interactive Sessions" tab.
  - Click on the red Delete button.



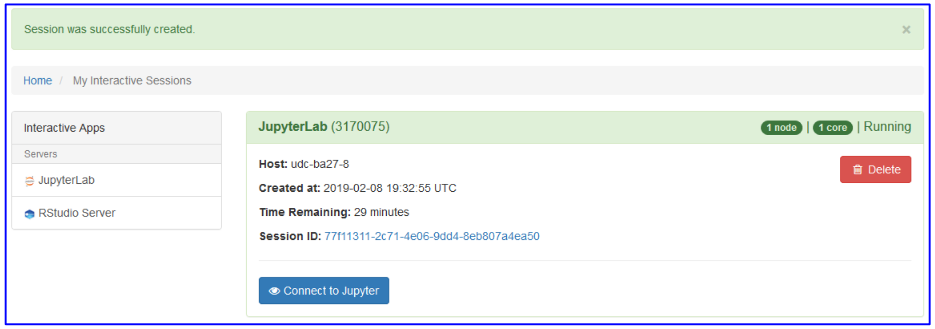
Tensor Flow with Keras

1. Load the Keras Packages

```
from keras.models import Sequential
from keras.layers import Dense, Dropout
from keras.utils import to_categorical
from keras.optimizers import SGD
```

2. Read in the Data

```
import numpy as np
data_file = '../Data/cancer_data.csv'
target_file = '../Data/cancer_target.csv'
cancer_data = np.loadtxt(data_file, dtype=float, delimiter=',')
cancer_target = np.loadtxt(target_file, dtype=int, delimiter=',')
```



Session was successfully created.

JupyterLab (3170075) | Running

Host: udc-ba27-8
Created at: 2019-02-08 19:32:55 UTC
Time Remaining: 29 minutes
Session ID: 77f11311-2c71-4e06-9dd4-8eb807a4ea50

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NEED MORE HELP?

<u>Office Hours</u>

Tuesdays:	3 pm - 5 pm, PLSB 430
Thursdays:	10 am - noon, HSL, downstairs
Thursdays:	3 pm - 5 pm, PLSB 430

Website:

arcs.Virginia.edu

Or, for immediate help:

hpc-support@virginia.edu

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