JUPYTERHUB, PYTHON, CONTAINERS & MORE:

INTRO TO USING POPULAR OPEN SOURCE TOOLS ON LC

PRESENTED BY

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REASON FOR THIS WORKSHOP

- Working with your favorite software/apps/tools/ languages/packages/etc. is different in a cluster/HPC/ shared environment than on a desktop!
- We want to give you a few different options for smoothing out your workflow and getting access to the tools you want!

AGENDA

- A few popular open source languages
  - **Python** on LC
    - Python virtual environments
    - How to install python packages: pytorch, tensorflow
  - **Julia** on LC
  - **R** on LC
- **JupyterHub** (out of the box & with custom kernels)
- How to use **containers**
- How to use **spack**, a package manager
- How to know what you can install

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HAVE YOU USED PYTHON BEFORE?

A. Yes, a lot

B. Yes, a little

C. Not yet

USING PYTHON ON LC

Use module system to use the python version of your choice!

```
janeh@flash21:~$ which python3
/usr/tce/bin/python3
janeh@flash21:~$ module avail python

------------------------- /usr/tce/modulefiles/Core --------------------------
   python/2.7.11    python/2.7.16 (D)    python/3.6.4
   python/2.7.13    python/3.5.1         python/3.7.2
   python/2.7.14    python/3.6.0         python/3.8.2

  Where:
   D:  Default Module

Use "module spider" to find all possible modules and extensions.
Use "module keyword key1 key2 ..." to search for all possible modules matching
any of the "keys".


janeh@flash21:~$ module load python/3.8.2
janeh@flash21:~$ which python3
/usr/tce/packages/python/python-3.8.2/bin/python3
```

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PYTHON VIRTUAL ENVIRONMENTS

`virtualenv` binary associated with the python module you've loaded is in your path now.

```
janeh@flash21:~$ which python3
/usr/tce/packages/python/python-3.8.2/bin/python3
janeh@flash21:~$ which virtualenv
/usr/tce/packages/python/python-3.8.2/bin/virtualenv
```

You can create your own virtual environment via `virtualenv –system-site-package <venv_dir_path>`

```
janeh@flash21:~$ virtualenv --system-site-package ~/myvenv
Using base prefix '/collab/usr/gapps/python/build/spack-toss3.4/opt/spack/linux-rhel7-ivyb
ridge/gcc-4.9.3/python-3.8.2-6me27g5yfvrxpcsemax25kovzjbf22vt'
New python executable in /g/g0/janeh/myvenv/bin/python3.8
Also creating executable in /g/g0/janeh/myvenv/bin/python
Installing setuptools, pip, wheel...
done.
```

https://hpc.llnl.gov/software/development-environment-software/python

PYTHON VIRTUAL ENVIRONMENTS

Your newly created virtual environment has its own python binaries, pip (package manager), etc.

This is an environment **you** can edit!

To start working with your virtual environment, you need to activate it via `source <venv_dir_path>/bin/activate`

```
janeh@flash21:~$ cd ~/myvenv
janeh@flash21:~/myvenv$ ls
bin  include  lib  lib64
janeh@flash21:~/myvenv$ ls bin
activate      activate.fish  activate.xsh      pip   pip3.8  python-config  python3.8
activate.csh  activate.ps1   activate_this.py  pip3  python  python3        wheel
janeh@flash21:~/myvenv$ which python3
/usr/tce/packages/python/python-3.8.2/bin/python3
janeh@flash21:~/myvenv$ source bin/activate
(myvenv) janeh@flash21:~/myvenv$ which python3
~/myvenv/bin/python3
```

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INSTALLING PYTHON PACKAGES — TENSORFLOW (X86)

Having created and activated your python virtual environment, you can now use your default `pip` to install tensorflow:

```
(myvenv) janeh@flash21:~/myvenv$ which pip
~/myvenv/bin/pip
(myvenv) janeh@flash21:~/myvenv$ pip install intel-tensorflow
```

INSTALLING PYTHON PACKAGES — TENSORFLOW (X86)

Having created and activated your python virtual environment, you can now use your default `pip` to install tensorflow:

```
(myvenv) janeh@flash21:~/myvenv$ which pip
~/myvenv/bin/pip
(myvenv) janeh@flash21:~/myvenv$ pip install intel-tensorflow
```

When I did this, I got a complaint about a dependency — nbformat:

```
ERROR: pip's dependency resolver does not currently take into account all the packages tha
t are installed. This behaviour is the source of the following dependency conflicts.
plotly 2.2.0 requires nbformat>=4.2, which is not installed.
```

Installing the correct version of nbformat fixed this:

```
(myvenv) janeh@flash21:~/myvenv$ pip install nbformat==4.2
```

INSTALLING PYTHON PACKAGES — TENSORFLOW (X86)

After installation, check you can import and use tensorflow:

```
(myvenv) janeh@flash21:~/myvenv$ python3
Python 3.8.2 (default, Mar 18 2020, 12:19:58)
[GCC 4.9.3] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow
>>> msg = tensorflow.constant("TensorFlow 2.0 Hello World")
2021-05-26 19:57:17.997095: I tensorflow/core/platform/cpu_feature_guard.cc:142] This Tens
orFlow binary is optimized with oneAPI Deep Neural Network Library (oneDNN) to use the fol
lowing CPU instructions in performance-critical operations:  AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate compiler flags
.
2021-05-26 19:57:18.000234: I tensorflow/core/common_runtime/process_util.cc:146] Creating
 new thread pool with default inter op setting: 2. Tune using inter_op_parallelism_threads
 for best performance.
>>> tensorflow.print(msg)
TensorFlow 2.0 Hello World
```

More docs on installation and testing @

https://lc.llnl.gov/confluence/display/LC/TensorFlow+in+LC

INSTALLING PYTHON PACKAGES — PYTORCH (X86)

Similarly, using your virtual environment's pip, install pytorch:

```
(myvenv) janeh@flash21:~/myvenv$ which pip
~/myvenv/bin/pip
(myvenv) janeh@flash21:~/myvenv$ pip install torch torchvision
```

INSTALLING PYTHON PACKAGES — PYTORCH (X86)

Similarly, using your virtual environment's pip, install pytorch:

```
(myvenv) janeh@flash21:~/myvenv$ which pip
~/myvenv/bin/pip
(myvenv) janeh@flash21:~/myvenv$ pip install torch torchvision
```

And check that installation is successful:

```
Successfully installed torch-1.8.1 torchvision-0.9.1
(myvenv) janeh@flash21:~/myvenv$ python3
Python 3.8.2 (default, Mar 18 2020, 12:19:58)
[GCC 4.9.3] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import torch
>>> x = torch.rand(5, 3)
>>> print(x)
tensor([[0.2729, 0.2918, 0.0528],
        [0.8790, 0.7048, 0.7278],
        [0.2984, 0.0410, 0.3625],
        [0.6315, 0.2937, 0.9328],
        [0.4661, 0.8340, 0.9212]])
```

https://lc.llnl.gov/confluence/display/LC/PyTorch+in+LC

INSTALLING PYTHON PACKAGES — SIERRA/LASSEN/RZANSEL


```
janeh@lassen708:/usr/workspace/janeh$ mkdir -p opence
janeh@lassen708:/usr/workspace/janeh$ tar -xzf /collab/usr/global/tools/openc
e/${SYS_TYPE}/opence.tar.gz -C opence
```

```
janeh@lassen708:/usr/workspace/janeh$ source opence/bin/activate
(opence) janeh@lassen708:/usr/workspace/janeh$ conda-unpack
```

```
(opence) janeh@lassen708:/usr/workspace/janeh$ python3
Python 3.7.10 (default, Feb 26 2021, 19:30:21)
[GCC 7.3.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import torch
>>> import tensorflow
2021-12-07 14:56:00.454139: I tensorflow/stream_executor/platform/default/dso
_loader.cc:49] Successfully opened dynamic library libcudart.so.10.2
```

https://lc.llnl.gov/confluence/display/LC/Deep+Learning+in+LC

https://lc.llnl.gov/confluence/display/LC/2021/03/08/Open-CE+for+Lassen

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HAVE YOU USED JULIA BEFORE?

A. Yes, a lot

B. Yes, a little

C. Not yet

USING JULIA ON LC


```
janeh@quartz2498:~$ which julia
/usr/gapps/julia/bin/julia
janeh@quartz1154:~$ cd /usr/gapps/julia/bin/
janeh@quartz1154:/usr/gapps/julia/bin$ ls
julia         julia-1.5.1         julia-1.6.1-power  julia-1.6.3-power
julia-0.6     julia-1.5.3         julia-1.6.2        julia-power
julia-0.7     julia-1.5.3-power   julia-1.6.2-power
julia-1.2.0   julia-1.6.1         julia-1.6.3
janeh@quartz1154:/usr/gapps/julia/bin$ ls -l julia
lrwxrwxrwx 1 janeh janeh 31 Oct  8 16:10 julia -> ../julia-1.6.3-x86-64/bin/j
ulia
janeh@quartz1154:/usr/gapps/julia/bin$ ls -l julia-power
lrwxrwxrwx 1 janeh janeh 27 Oct 11 10:12 julia-power -> ../julia-1.6.3-power9
/julia
```

To add this directory to your PATH:

export PATH=$PATH:/usr/gapps/julia/bin *#bash*

setenv PATH $PATH:/usr/gapps/julia/bin *#csh*

USING JULIA ON LC


```
janeh@quartz1154:/usr/gapps/julia/bin$ ./julia
               _
   _       _ _(_)_     |  Documentation: https://docs.julialang.org
  (_)     | (_) (_)    |
   _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 1.6.3 (2021-09-23)
 _/ |\__'_|_|_|\__'_|  |  Official https://julialang.org/ release
|__/                   |

(@v1.6) pkg> add Example
    Updating registry at `~/.julia/registries/General`
    Updating git-repo `https://github.com/JuliaRegistries/General.git`
   Resolving package versions...
    Updating `~/.julia/environments/v1.6/Project.toml`
  [7876af07] + Example v0.5.3
    Updating `~/.julia/environments/v1.6/Manifest.toml`
  [7876af07] + Example v0.5.3
Precompiling project...
  1 dependency successfully precompiled in 3 seconds

julia> using Example

julia> hello("LLNL")
"Hello, LLNL"
```

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HAVE YOU USED R BEFORE?

A. Yes, a lot

B. Yes, a little

C. Not yet

USING R ON LC

R v3.6 lives on LC machines at `/usr/bin/R`:

```
janeh@flash21:~$ which R
/usr/bin/R
janeh@flash21:~$ R

R version 3.6.0 (2019-04-26) -- "Planting of a Tree"
Copyright (C) 2019 The R Foundation for Statistical Computing
Platform: x86_64-redhat-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

>
```

USING R ON LC

To customize your environment/add packages, `install.packages('<package name>')`.

```
> install.packages('IRkernel')
Installing package into '/usr/lib64/R/library'
(as 'lib' is unspecified)
Warning in install.packages("IRkernel") :
  'lib = "/usr/lib64/R/library"' is not writable
Would you like to use a personal library instead? (yes/No/cancel) y
Would you like to create a personal library
'~/R/x86_64-redhat-linux-gnu-library/3.6'
to install packages into? (yes/No/cancel) y
```

You'll be prompted to create a personal library where you can install packages – similar to how we created a virtual environment to install python packages.

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HAVE YOU USED JUPYTER NOTEBOOKS BEFORE?

A. Yes, a lot

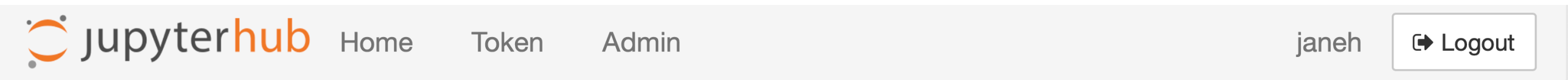
B. Yes, a little

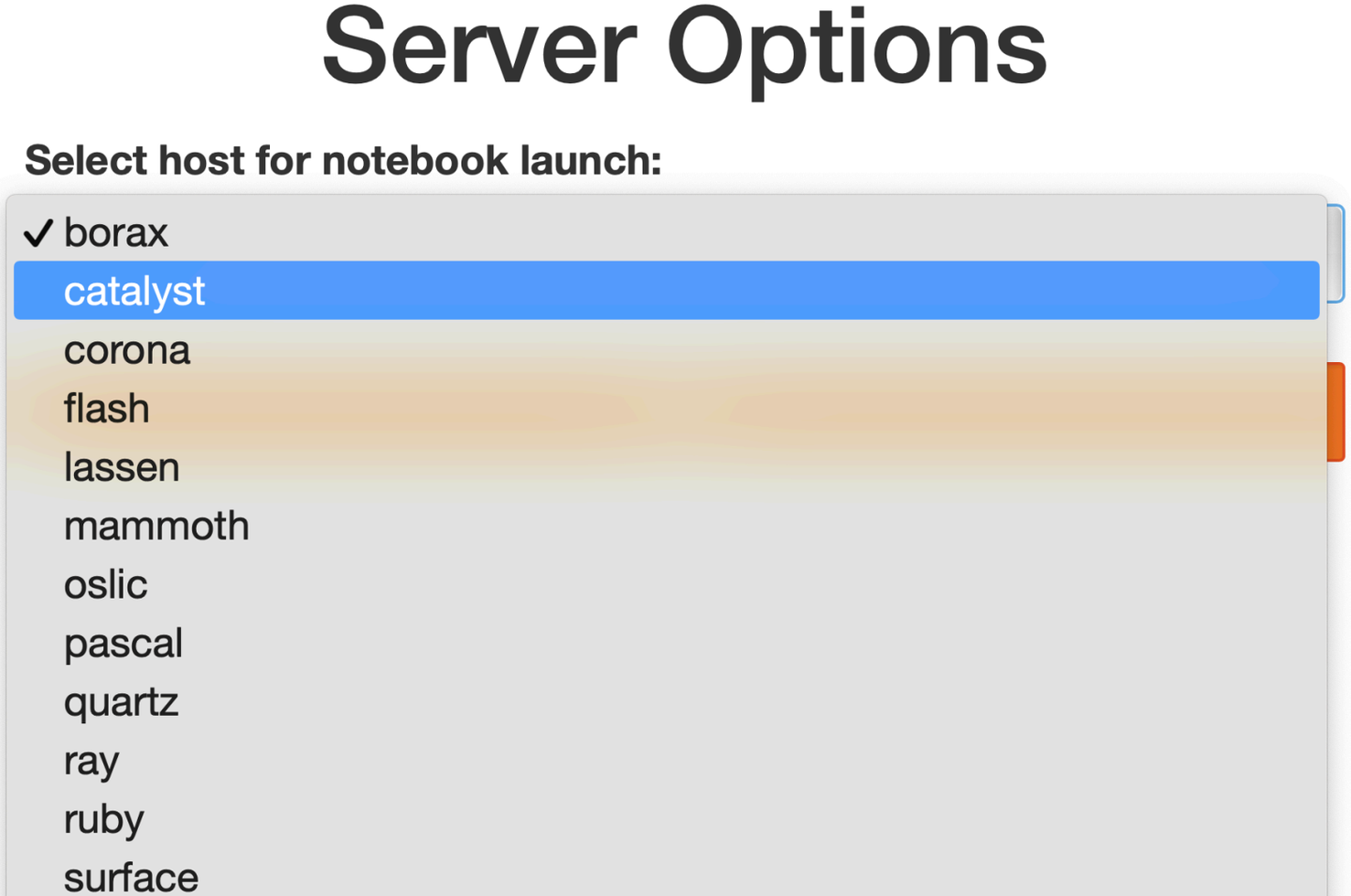
C. Not yet

USING JUPYTERHUB

On the CZ, log in to JupyterHub at https://lc.llnl.gov/jupyter

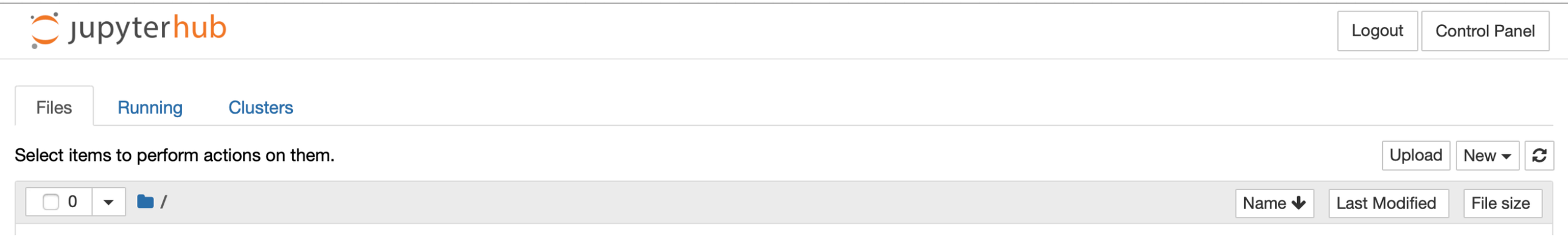
After authenticating with your pin and RSA token, you'll be taken to a screen where you can select a server.





USING JUPYTERHUB

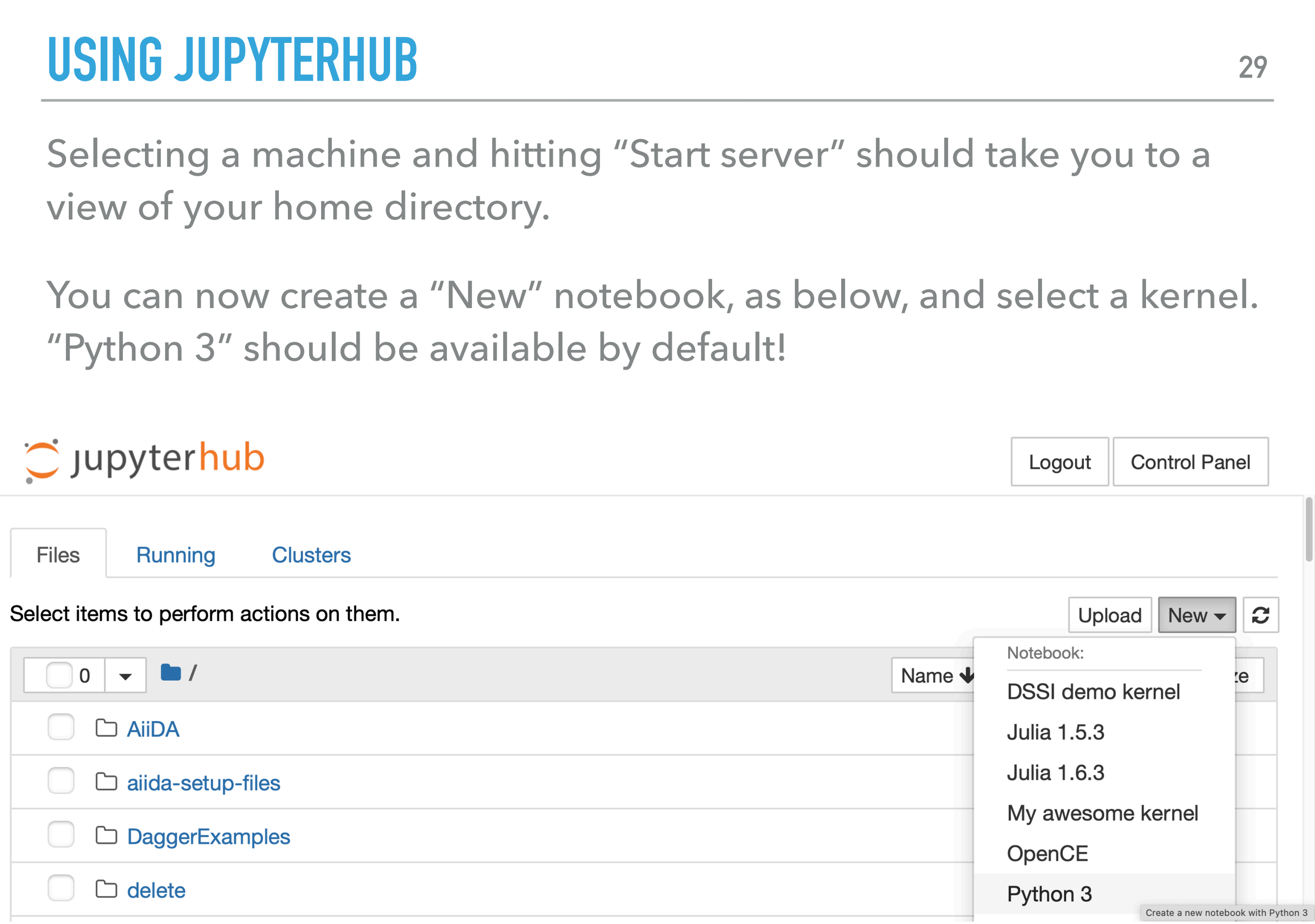
Selecting a machine and hitting “Start server” should take you to a view of your home directory with a heading like



USING JUPYTERHUB

Selecting a machine and hitting “Start server” should take you to a view of your home directory.

You can now create a “New” notebook, as below, and select a kernel. “Python 3” should be available by default!



USING JUPYTERHUB

See

https://hpc.llnl.gov/services/jupyter

for more info on JupyterHub!

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CUSTOM JUPYTERHUB KERNELS

We'll talk about creating custom kernels for:

- Python
- Julia
- R

For each of these, you'll need to:

- Install a package (ipykernel, IJulia, or IRkernel)
- Check for & possibly create `~/.local/share/jupyter/kernels/<Directory for custom kernel name>/kernel.json`

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CUSTOM JUPYTERHUB KERNELS: PYTHON

Install ipykernel into your python virtual environment:

```
janeh@flash21:~/myvenv$ source bin/activate
(myvenv) janeh@flash21:~/myvenv$ pip install ipykernel
```

CUSTOM JUPYTERHUB KERNELS: PYTHON

Install your custom kernel to .local in your home directory

```
(myvenv) janeh@flash21:~/myvenv$ python3 -m ipykernel install --prefix=$HOME/.local/ --name 'myve
nv_kernel' --display-name 'myvenv_kernel'
Installed kernelspec myvenv_kernel in /g/g0/janeh/.local/share/jupyter/kernels/myvenv_kernel
```

Check that a JSON file with expected format exists for your new kernel:

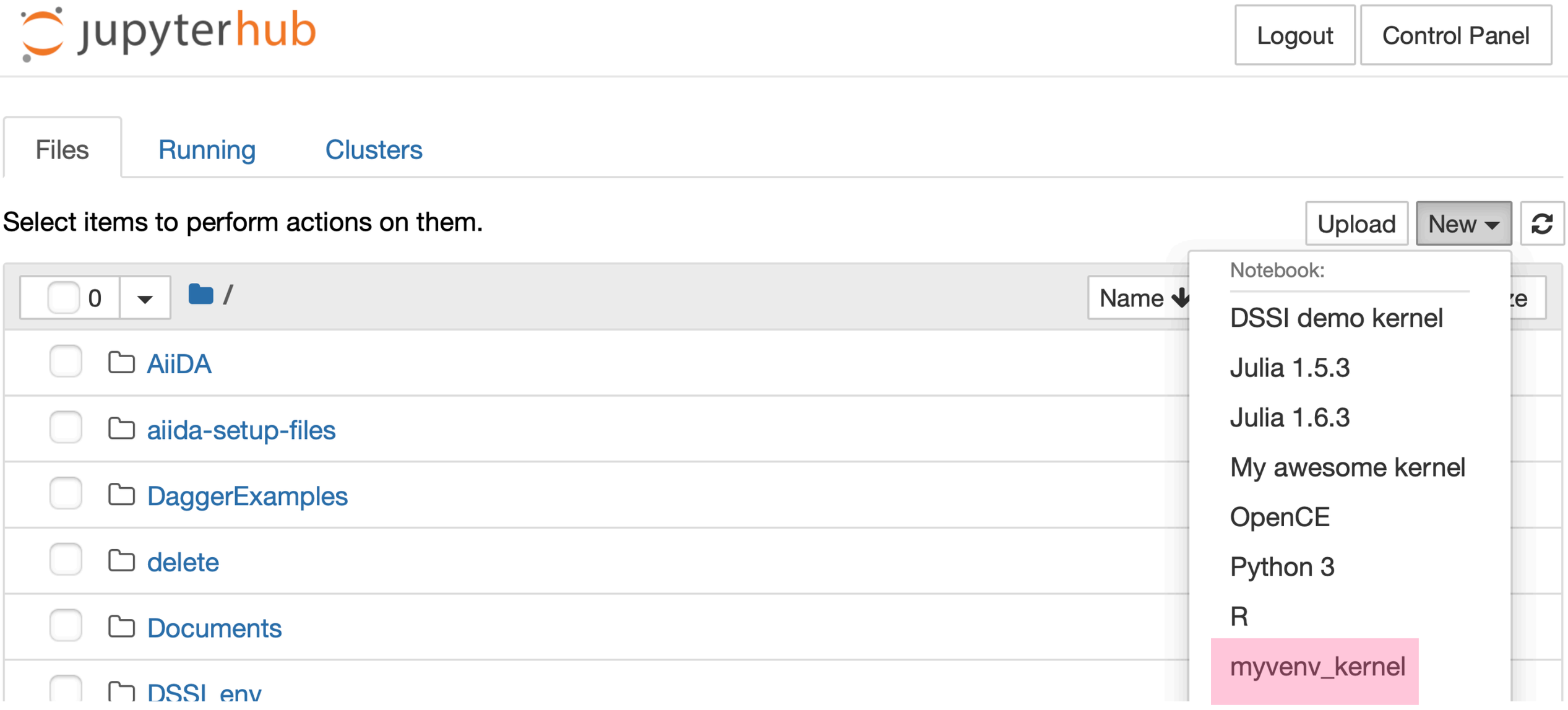
```
(myvenv) janeh@flash21:~/myvenv$ cd ~/.local/share/jupyter/kernels/
(myvenv) janeh@flash21:~/.local/share/jupyter/kernels$ ls
R  dssi-demo-kernel  julia-1.5  myvenv_kernel  testkernel
(myvenv) janeh@flash21:~/.local/share/jupyter/kernels$ cd myvenv_kernel/
(myvenv) janeh@flash21:~/.local/share/jupyter/kernels/myvenv_kernel$ ls
kernel.json  logo-32x32.png  logo-64x64.png
(myvenv) janeh@flash21:~/.local/share/jupyter/kernels/myvenv_kernel$ cat kernel.json
{
 "argv": [
  "/g/g0/janeh/myvenv/bin/python3",
  "-m",
  "ipykernel_launcher",
  "-f",
  "{connection_file}"
 ],
 "display_name": "myvenv_kernel",
 "language": "python"
}(myvenv) janeh@flash21:~/.local/share/jupyter/kernels/myvenv_kernel$
```

CUSTOM JUPYTERHUB KERNELS: PYTHON

Now, go to JupyterHub and check

(1) you can access the new kernel

(2) the kernel has any packages you installed to that virtual environment

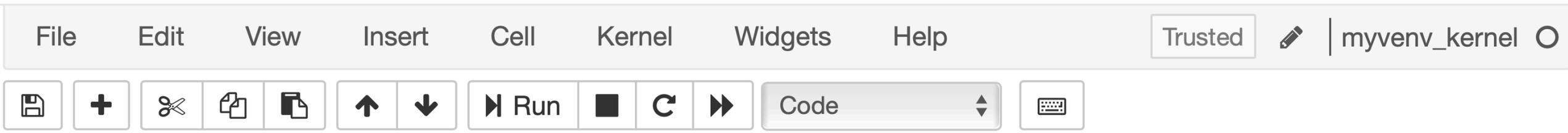


CUSTOM JUPYTERHUB KERNELS: PYTHON

Now, go to JupyterHub and check

(1) you can access the new kernel

(2) the kernel has any packages you installed to that virtual environment




```
In [1]: import torch
        import tensorflow

In [2]: msg = tensorflow.constant("Another hello world");
        tensorflow.print(msg)

        Another hello world

In [3]: torch.rand(3,3)

Out[3]: tensor([[0.8326, 0.7758, 0.8238],
                [0.7299, 0.2683, 0.5755],
                [0.5272, 0.9425, 0.7744]])
```

CUSTOM JUPYTERHUB KERNELS: PYTHON

See the sections on custom kernels and home directory installation at

https://hpc.llnl.gov/services/jupyter

for more info!

CUSTOM JUPYTERHUB KERNELS

We'll talk about creating custom kernels for:

- Python
- **Julia**
- R

For each of these, you'll need to:

- Install a package (ipykernel, IJulia, or IRkernel)
- Check for & possibly create `~/.local/share/jupyter/kernels/<Directory for custom kernel name>/kernel.json`

CUSTOM JUPYTERHUB KERNELS: JULIA

First, install IJulia:

```
janeh@oslic7:~$ julia
               _
   _       _ _(_)_     |  Documentation: https://docs.julialang.org
  (_)     | (_) (_)    |
   _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 1.6.3 (2021-09-23)
 _/ |\__'_|_|_|\__'_|  |  Official https://julialang.org/ release
|__/                   |

(@v1.6) pkg> add IJulia
    Updating registry at `~/.julia/registries/General`
    Updating git-repo `https://github.com/JuliaRegistries/General.git`
   Resolving package versions...
   Installed VersionParsing ─ v1.2.1
   Installed ZeroMQ_jll ──── v4.3.4+0
   Installed libsodium_jll ─ v1.0.20+0
   Installed Conda ────────── v1.6.0
   Installed Parsers ──────── v2.1.2
   Installed JSON ─────────── v0.21.2
  Downloaded artifact: libsodium
  Downloaded artifact: ZeroMQ
    Updating `~/.julia/environments/v1.6/Project.toml`
  [7073ff75] + IJulia v1.23.2
    Updating `~/.julia/environments/v1.6/Manifest.toml`
```

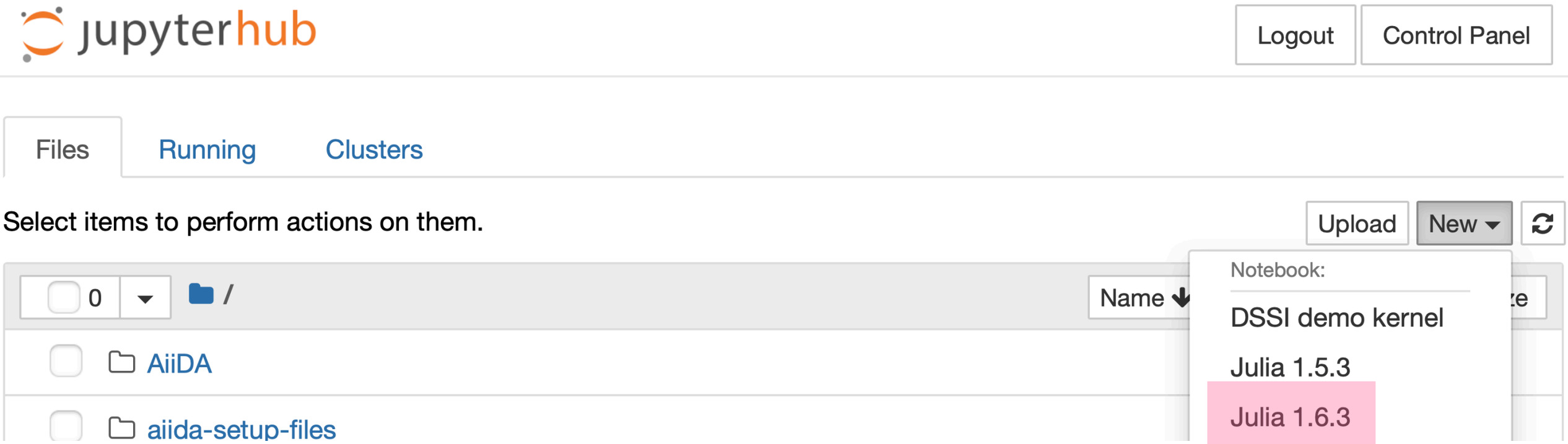
CUSTOM JUPYTERHUB KERNELS: JULIA

Go to `$HOME/.local/share/jupyter/kernels`

```
janeh@oslic7:~/.local/share/jupyter/kernels$ ls
R                 julia-1.5    myvenv_kernel  spack-R
dssi-demo-kernel  julia-1.6.3  opence         testkernel
janeh@oslic7:~/.local/share/jupyter/kernels$ ls julia-1.6.3/
kernel.json
janeh@oslic7:~/.local/share/jupyter/kernels$ cat julia-1.6.3/kernel.json
{
  "display_name": "Julia 1.6.3",
  "argv": [
    "/collab/usr/gapps/julia/julia-1.6.3-x86-64/bin/julia",
    "-i",
    "--color=yes",
    "--project=@.",
    "/g/g0/janeh/.julia/packages/IJulia/e8kqU/src/kernel.jl",
    "{connection_file}"
  ],
  "language": "julia",
  "env": {},
  "interrupt_mode": "signal"
}
```

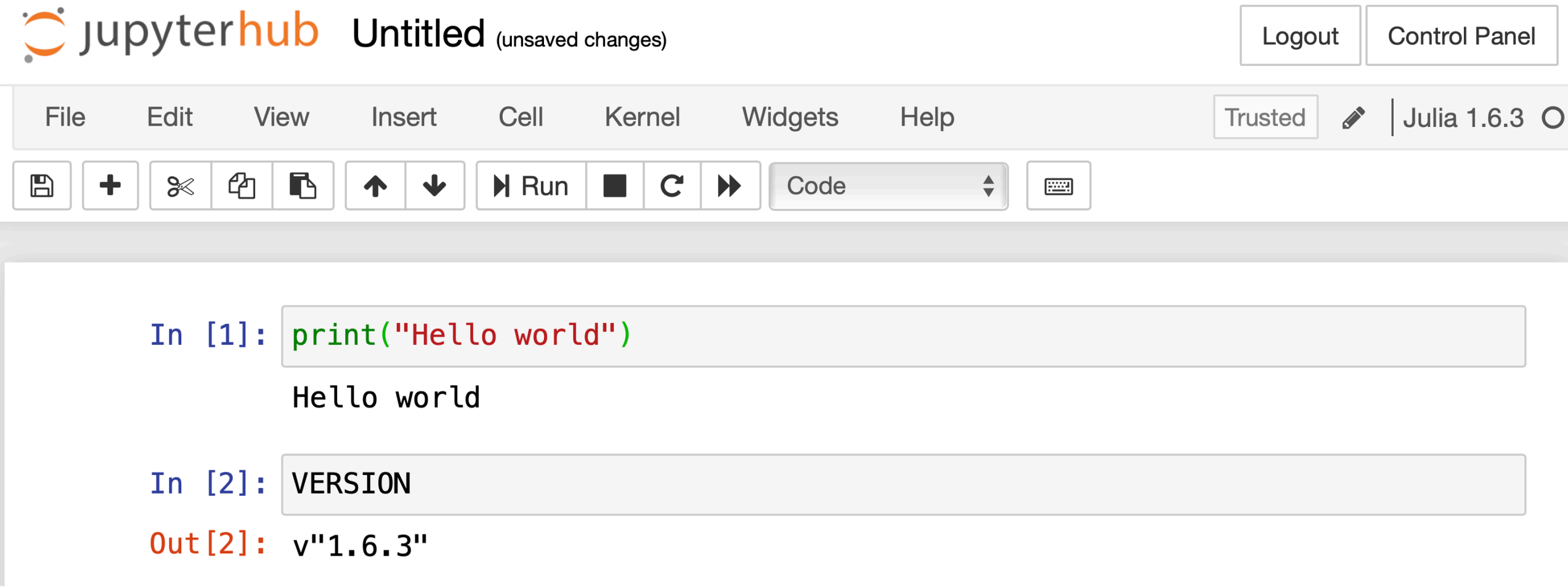
CUSTOM JUPYTERHUB KERNELS: JULIA

Once you've checked `kernel.json` exists for the desired version of Julia, the Julia kernel will be visible on JupyterHub:



CUSTOM JUPYTERHUB KERNELS: JULIA

Selecting your new custom kernel, you can open a Julia notebook:



CUSTOM JUPYTERHUB KERNELS

We'll talk about creating custom kernels for:

- Python
- Julia
- **R**

For each of these, you'll need to:

- Install a package (ipykernel, IJulia, or IRkernel)
- Check for & possibly create `~/.local/share/jupyter/kernels/<Directory for custom kernel name>/kernel.json`

CUSTOM JUPYTERHUB KERNELS: R

First, fire up the default R on LC:

```
janeh@flash21:~$ which R
/usr/bin/R
janeh@flash21:~$ R

R version 3.6.0 (2019-04-26) -- "Planting of a Tree"
Copyright (C) 2019 The R Foundation for Statistical Computing
Platform: x86_64-redhat-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

>
```

CUSTOM JUPYTERHUB KERNELS: R

Install IRKernel via `install.packages('IRkernel')`:

```
> install.packages('IRkernel')
Installing package into '/usr/lib64/R/library'
(as 'lib' is unspecified)
Warning in install.packages("IRkernel") :
  'lib = "/usr/lib64/R/library"' is not writable
Would you like to use a personal library instead? (yes/No/cancel) y
Would you like to create a personal library
'~/R/x86_64-redhat-linux-gnu-library/3.6'
to install packages into? (yes/No/cancel) y
```

You'll be prompted to create a personal library where you can install packages – similar to how we created a virtual environment to install python packages.

CUSTOM JUPYTERHUB KERNELS: R

You'll next be prompted to select a "CRAN mirror", a web server from which to download IRkernel. (I chose #75.)

```
--- Please select a CRAN mirror for use in this session ---
Secure CRAN mirrors

 1: 0-Cloud [https]
 2: Australia (Canberra) [https]
 3: Australia (Melbourne 1) [https]
 4: Australia (Melbourne 2) [https]
 5: Australia (Perth) [https]
 6: Austria [https]
 7: Brazil (BA) [https]
```

```
75: USA (OR) [https]
76: USA (TN) [https]
77: USA (TX 1) [https]
78: Uruguay [https]
79: (other mirrors)

Selection: 75
trying URL 'https://ftp.osuosl.org/pub/cran/src/contrib/IRkernel_1.2.tar.gz'
Content type 'application/x-gzip' length 62663 bytes (61 KB)
==================================================
downloaded 61 KB
```

CUSTOM JUPYTERHUB KERNELS: R

Create a new directory called `.local/share/jupyter/kernels/R`

```
janeh@flash21:~$ mkdir .local/share/jupyter/kernels/R/
```

CUSTOM JUPYTERHUB KERNELS: R

Create a new directory called `.local/share/jupyter/kernels/R`

```
janeh@flash21:~$ mkdir .local/share/jupyter/kernels/R/
```

where you will create a file, `kernel.json`

```
janeh@flash21:~$ cd .local/share/jupyter/kernels/R/
janeh@flash21:~/.local/share/jupyter/kernels/R$ touch kernel.json
```

CUSTOM JUPYTERHUB KERNELS: R

Create a new directory called `.local/share/jupyter/kernels/R`

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janeh@flash21:~$ mkdir .local/share/jupyter/kernels/R/
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where you will create a file, `kernel.json`

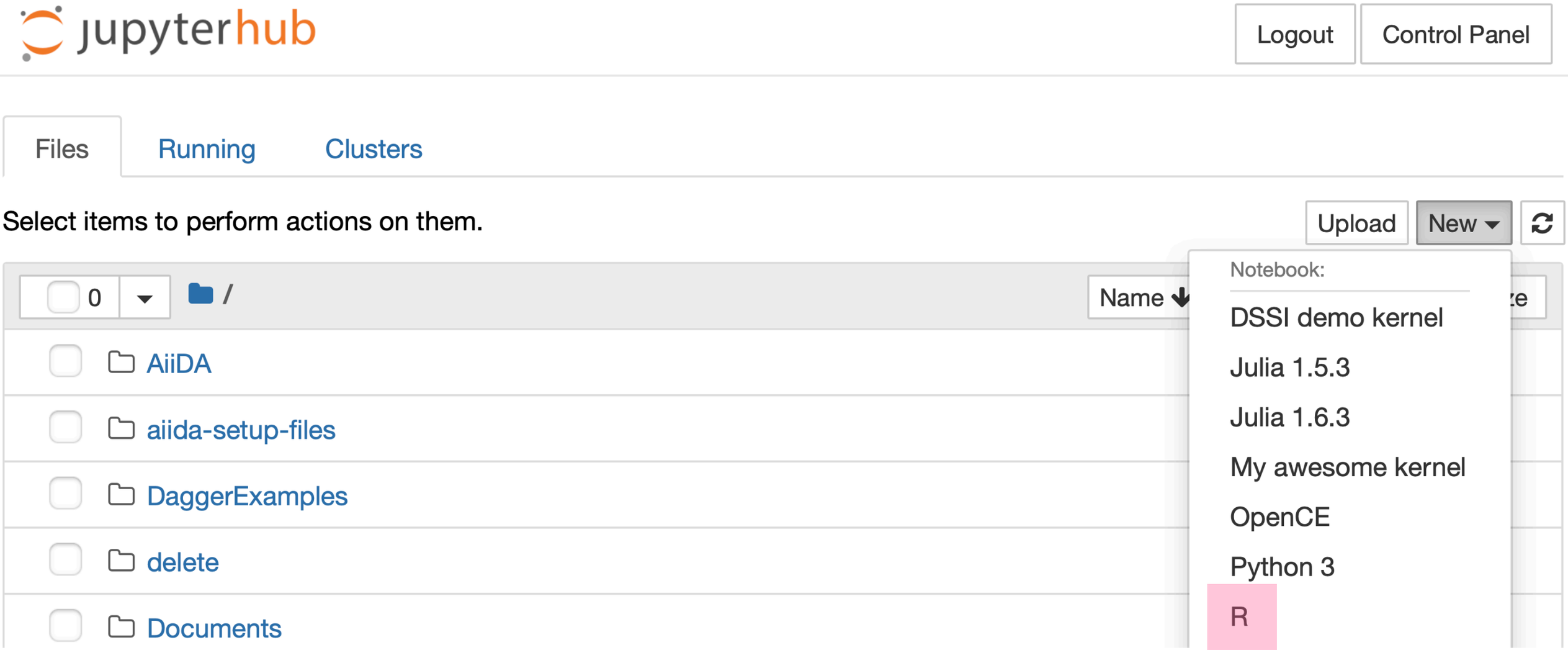
```
janeh@flash21:~$ cd .local/share/jupyter/kernels/R/
janeh@flash21:~/.local/share/jupyter/kernels/R$ touch kernel.json
```

and populate it with the following information:

```
janeh@flash21:~/.local/share/jupyter/kernels/R$ cat kernel.json
{"argv": ["/usr/bin/R", "--quiet", "-e", "IRkernel::main()", "--args", "{connection_file}"],
 "display_name":"R",
 "language":"R"
}
```

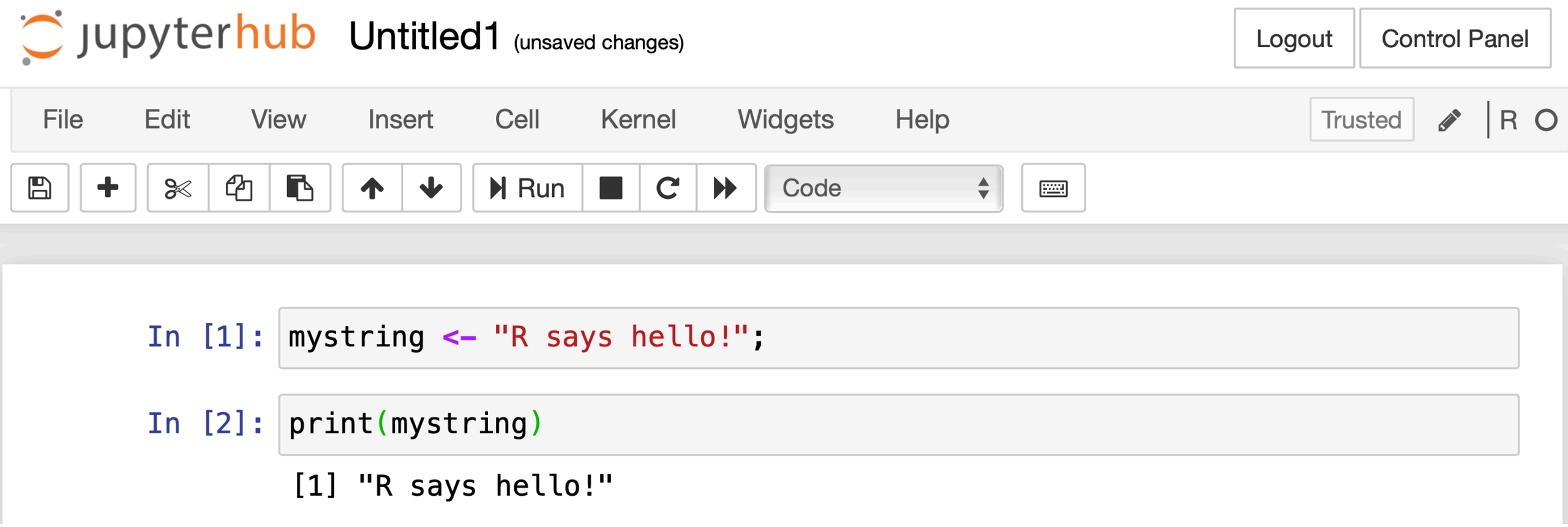
CUSTOM JUPYTERHUB KERNELS: R

Now, go to JupyterHub and check that you can use R!



CUSTOM JUPYTERHUB KERNELS: R

Now, go to JupyterHub and check that you can use R!



https://hpc.llnl.gov/services/Jupyter/R

AGENDA

- A few popular open source languages
  - Python on LC
    - Python virtual environments
    - How to install python packages: pytorch, tensorflow
  - Julia on LC
  - R on LC
- JupyterHub (out of the box & with custom kernels)
- **How to use containers**
- How to use spack, a package manager
- How to know what you can install

HAVE YOU WORKED WITH CONTAINERS (LIKE DOCKER) BEFORE? 54

A. Yes, a lot

B. Yes, a little

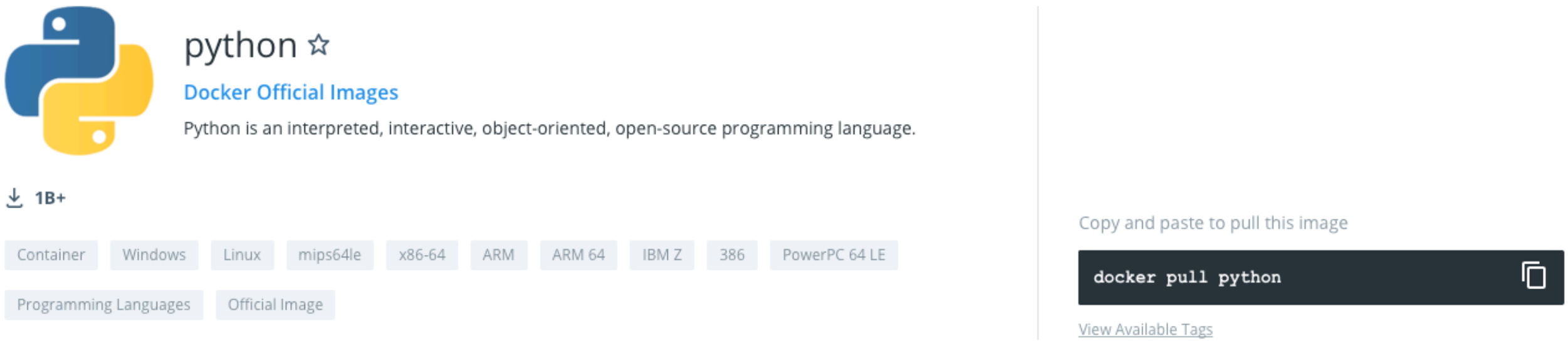
C. Not yet

USING CONTAINERS

You can use containers to work with an application that isn't installed/supported on LC machines, without needing to install the app yourself.

LC uses Singularity rather than Docker to run containers, but your Docker containers will work with Singularity!

For example, say you want the latest python available here:



USING CONTAINERS

python ☆

Docker Official Images

Python is an interpreted, interactive, object-oriented, open-source programming language.

1B+

Container | Windows | Linux | mips64le | x86-64 | ARM | ARM 64 | IBM Z | 386 | PowerPC 64 LE

Programming Languages | Official Image

Copy and paste to pull this image

```
docker pull python
```

View Available Tags

`singularity pull <name_for_container_img> docker://<name_from_dockerhub>`

```
janeh@flash21:~/Singularity/DSSI$ singularity pull mypython.img docker://python
INFO:    Converting OCI blobs to SIF format
INFO:    Starting build...
Getting image source signatures
```

Creates a file, `<name_for_container_img>`

```
janeh@flash21:~/Singularity/DSSI$ ls
mypython.img
```

USING CONTAINERS

You can “shell into” a container, allowing you to work with whatever binaries/apps live inside:

```
janeh@flash21:~/Singularity/DSSI$ which python3
/usr/tce/bin/python3
janeh@flash21:~/Singularity/DSSI$ python3
Python 3.7.2 (default, Feb 26 2019, 08:59:10)
[GCC 4.9.3] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> exit()
janeh@flash21:~/Singularity/DSSI$ singularity shell mypython.img bash
Singularity> which python3
/usr/local/bin/python3
Singularity> python3
Python 3.9.5 (default, May 12 2021, 15:26:36)
[GCC 8.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

USING CONTAINERS

When you're "in" the container, you can use the container apps but access your local filesystem*

```
janeh@flash21:~/Singularity/DSSI$ singularity shell mypython.img bash
Singularity> ls
mypython.img
Singularity> pwd
/g/g0/janeh/Singularity/DSSI
Singularity> echo $HOME
/g/g0/janeh
```

*Your home directory is viewable by default, but you have to explicitly "mount" other LC file systems. See the docs!

USING CONTAINERS

Without “entering” the container, you can execute commands as if you were inside the container with

`singularity exec <container> <command to run inside container>`

```
janeh@flash21:~/Singularity/DSSI$ singularity exec mypython.img python3 -c 'print("hello!")'
hello!
```

USING CONTAINERS

Similarly, you could work with R v4.1.0 using a container:

```
janeh@flash21:~/Singularity/DSSI$ singularity pull myR.img docker://r-base
```

USING CONTAINERS

Similarly, you could work with R v4.1.0 using a container:

```
janeh@flash21:~/Singularity/DSSI$ singularity pull myR.img docker://r-base
```

```
janeh@flash21:~/Singularity/DSSI$ singularity shell myR.img bash
Singularity> R

R version 4.1.0 (2021-05-18) -- "Camp Pontanezen"
Copyright (C) 2021 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

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  Natural language support but running in an English locale

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'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> msg <- "Hello!"
> print(msg)
```

USING CONTAINERS

See

https://lc.llnl.gov/cloud/services/Singularity/

for our docs with more examples.

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- How to know what you can install

USING SPACK

Can find docs and tutorials at

https://spack.readthedocs.io/en/latest/getting_started.html

As well as a list of all available packages at

https://spack.readthedocs.io/en/latest/package_list.html#r-irkernel

USING SPACK

First, install Spack with `git clone…`

```
janeh@flash21:~$ git clone https://github.com/spack/spack.git
Cloning into 'spack'...
remote: Enumerating objects: 283370, done.
remote: Counting objects: 100% (419/419), done.
remote: Compressing objects: 100% (249/249), done.
remote: Total 283370 (delta 134), reused 324 (delta 73), pack-reused 282951
Receiving objects: 100% (283370/283370), 114.64 MiB | 27.24 MiB/s, done.
Resolving deltas: 100% (120374/120374), done.
Updating files: 100% (8162/8162), done.
```

USING SPACK

First, install Spack with `git clone…`

Source your Spack environment to configure paths.

```
janeh@flash21:~$ git clone https://github.com/spack/spack.git
Cloning into 'spack'...
remote: Enumerating objects: 283370, done.
remote: Counting objects: 100% (419/419), done.
remote: Compressing objects: 100% (249/249), done.
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Resolving deltas: 100% (120374/120374), done.
Updating files: 100% (8162/8162), done.
janeh@flash21:~$ cd spack/share/spack/
janeh@flash21:~/spack/share/spack$ . setup-env.sh
```

USING SPACK

And then you're ready to install packages!

`spack install <packagename>`

```
janeh@flash21:~$ git clone https://github.com/spack/spack.git
Cloning into 'spack'...
remote: Enumerating objects: 283370, done.
remote: Counting objects: 100% (419/419), done.
remote: Compressing objects: 100% (249/249), done.
remote: Total 283370 (delta 134), reused 324 (delta 73), pack-reused 282951
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janeh@flash21:~$ cd spack/share/spack/
janeh@flash21:~/spack/share/spack$ . setup-env.sh
janeh@flash21:~/spack/share/spack$ spack install r
```

Often this will be enough to get a clean installation.

USING SPACK

Here, Spack complained about my compiler (gcc) version:

```
janeh@flash21:~$ git clone https://github.com/spack/spack.git
Cloning into 'spack'...
remote: Enumerating objects: 283370, done.
remote: Counting objects: 100% (419/419), done.
remote: Compressing objects: 100% (249/249), done.
remote: Total 283370 (delta 134), reused 324 (delta 73), pack-reused 282951
Receiving objects: 100% (283370/283370), 114.64 MiB | 27.24 MiB/s, done.
Resolving deltas: 100% (120374/120374), done.
Updating files: 100% (8162/8162), done.
janeh@flash21:~$ cd spack/share/spack/
janeh@flash21:~/spack/share/spack$ . setup-env.sh
janeh@flash21:~/spack/share/spack$ spack install r
==> Error: Conflicts in concretized spec "r@4.1.0%gcc@4.9.3~X~external-lapack~memory_profiling~rm
ath arch=linux-rhel7-haswell/zufij6s"
List of matching conflicts for spec:

    icu4c@67.1%gcc@4.9.3 cxxstd=11 arch=linux-rhel7-haswell
        ^python@3.8.10%gcc@4.9.3+bz2+ctypes+dbm~debug+libxml2+lzma~nis~optimizations+pic+pyexpat+
pythoncmd+readline+shared+sqlite3+ssl~tix~tkinter~ucs4+uuid+zlib patches=0d98e93189bc278fbc37a50e
d7f183bd8aaf249a8e1670a465f0db6bb4f8cf87 arch=linux-rhel7-haswell
```

USING SPACK

To fix this, I used the module system to find and load a newer version of gcc:

```
janeh@flash21:~/spack/share/spack$ module avail gcc

---------------------------------- /usr/tce/modulefiles/Core ----------------------------------
   gcc/4.8-redhat         gcc/6.1.0    gcc/7.3.0    gcc/8.3.1    gcc/10.2.1
   gcc/4.9.3      (D)     gcc/7.1.0    gcc/8.1.0    gcc/9.3.1

  Where:
   D:  Default Module

Use "module spider" to find all possible modules and extensions.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the
"keys".


janeh@flash21:~/spack/share/spack$ module load gcc/10.2.1

Lmod is automatically replacing "intel/19.0.4" with "gcc/10.2.1".


Due to MODULEPATH changes, the following have been reloaded:
  1) mvapich2/2.3
```

USING SPACK

I then registered the new compiler (version 10.2.1 of gcc) and used the syntax

`spack install <package> %<compiler_name>@<compiler_version>`

```
janeh@flash21:~/spack/share/spack$ spack compiler find
==> Added 1 new compiler to /g/g0/janeh/.spack/linux/compilers.yaml
    gcc@10.2.1
==> Compilers are defined in the following files:
    /g/g0/janeh/.spack/linux/compilers.yaml
janeh@flash21:~/spack/share/spack$ spack install r %gcc@10.2.1
```

USING SPACK

After this, R version 4.1.0 installed successfully.

With `spack find` I can see both what's installed and where.

```
janeh@flash21:~$ spack find
==> 29 installed packages
-- linux-rhel7-haswell / gcc@10.2.1 ----------------------------
berkeley-db@18.1.40  gettext@0.21   libmd@1.0.3          pcre2@10.36    sqlite@3.35.5
bzip2@1.0.8          icu4c@67.1     libunistring@0.9.10  perl@5.32.1    tar@1.34
curl@7.76.1          libbsd@0.11.3  libxml2@2.9.10       pkgconf@1.7.4  util-linux-uuid@2.36.2
diffutils@3.7        libffi@3.3     ncurses@6.2          python@3.8.10  xz@5.2.5
expat@2.3.0          libiconv@1.16  openjdk@11.0.8_10    r@4.1.0        zlib@1.2.11
gdbm@1.19            libidn2@2.3.0  openssl@1.1.1k       readline@8.1
janeh@flash21:~$ spack find r
==> 1 installed package
-- linux-rhel7-haswell / gcc@10.2.1 ----------------------------
r@4.1.0
janeh@flash21:~$ spack find --paths r
==> 1 installed package
-- linux-rhel7-haswell / gcc@10.2.1 ----------------------------
r@4.1.0  /g/g0/janeh/spack/opt/spack/linux-rhel7-haswell/gcc-10.2.1/r-4.1.0-kr3ugnzx2qmoggyeti4ce
pjzx7n3i4yp
```

USING SPACK

`spack load <package>` allows me to find my new package:

```
janeh@flash21:~$ which R
/usr/bin/R
janeh@flash21:~$ spack load r
janeh@flash21:~$ which R
~/spack/opt/spack/linux-rhel7-haswell/gcc-10.2.1/r-4.1.0-kr3ugnzx2qmoggyeti4cepjzx7n3i4yp/bin/R
janeh@flash21:~$ R

R version 4.1.0 (2021-05-18) -- "Camp Pontanezen"
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Platform: x86_64-pc-linux-gnu (64-bit)

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>
```

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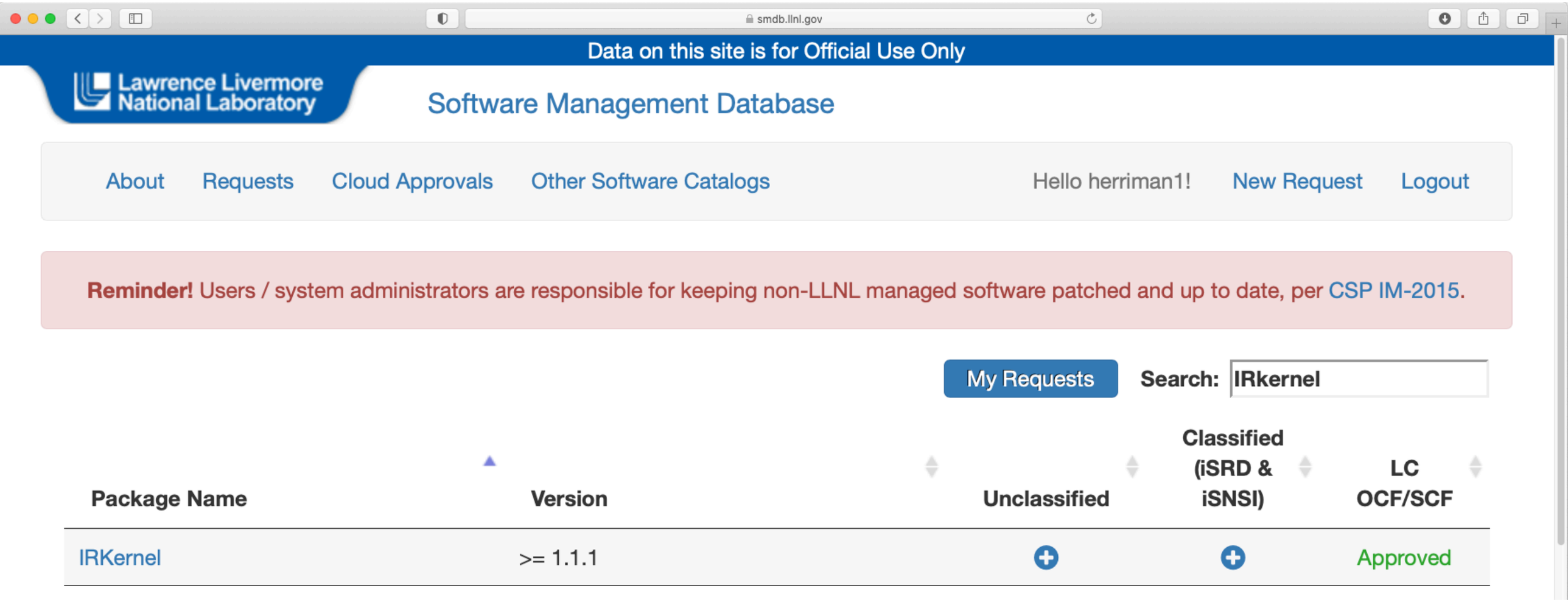
- **How to know what you can install**

WHAT YOU CAN INSTALL

See SMDB for prior approvals (https://smdb.llnl.gov/) and reach out to the hotline if you're unsure (lc-hotline@llnl.gov)



WHAT YOU CAN INSTALL

Additionally, any python packages in wheelhouse are approved:

https://www-lc.llnl.gov/python/wheelhouse/

Over 1100 packages, including multiple versions.

DISCLAIMER