

CIML Summer Institute:

Running Secure Jupyter Notebooks on Expanse

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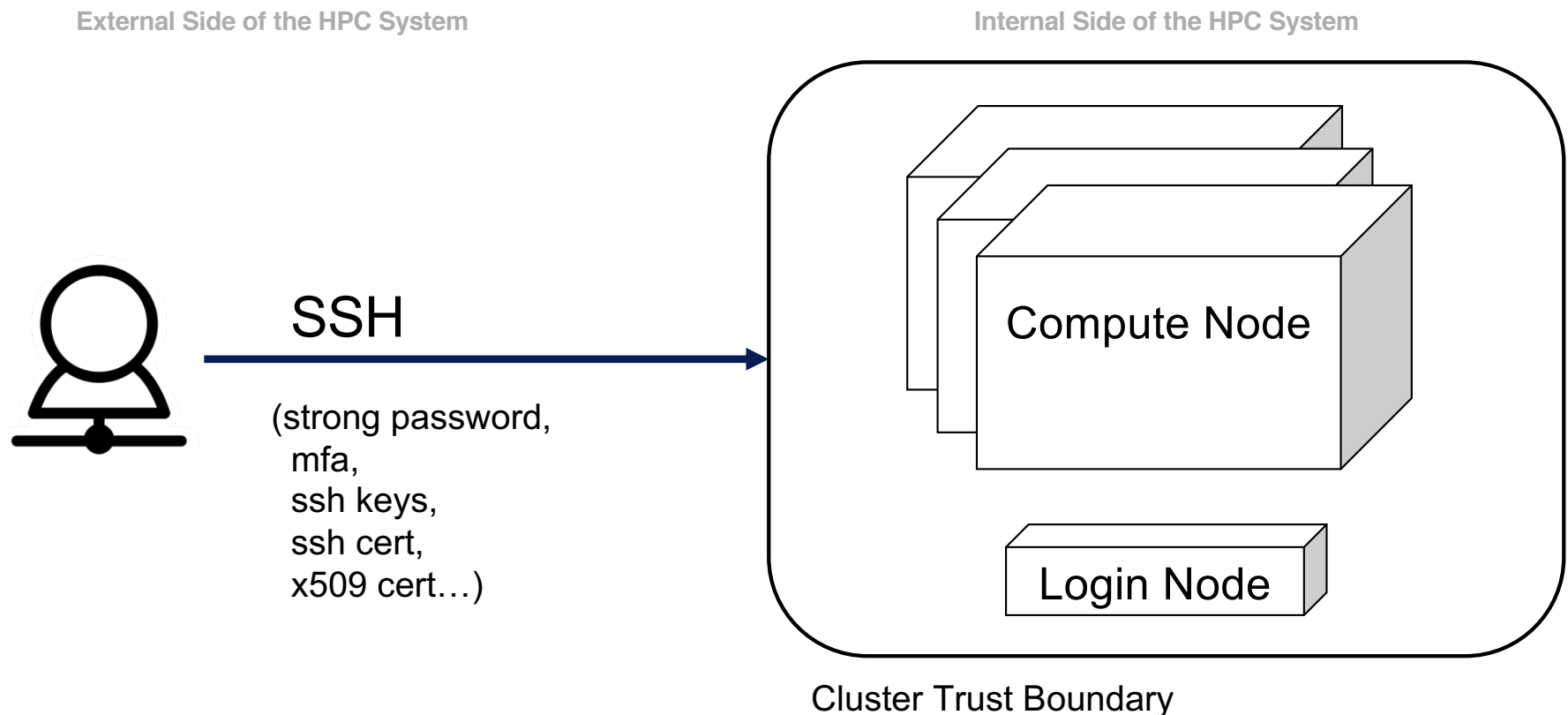
EXPANSE
COMPUTING WITHOUT BOUNDARIES

SAN DIEGO SUPERCOMPUTER CENTER

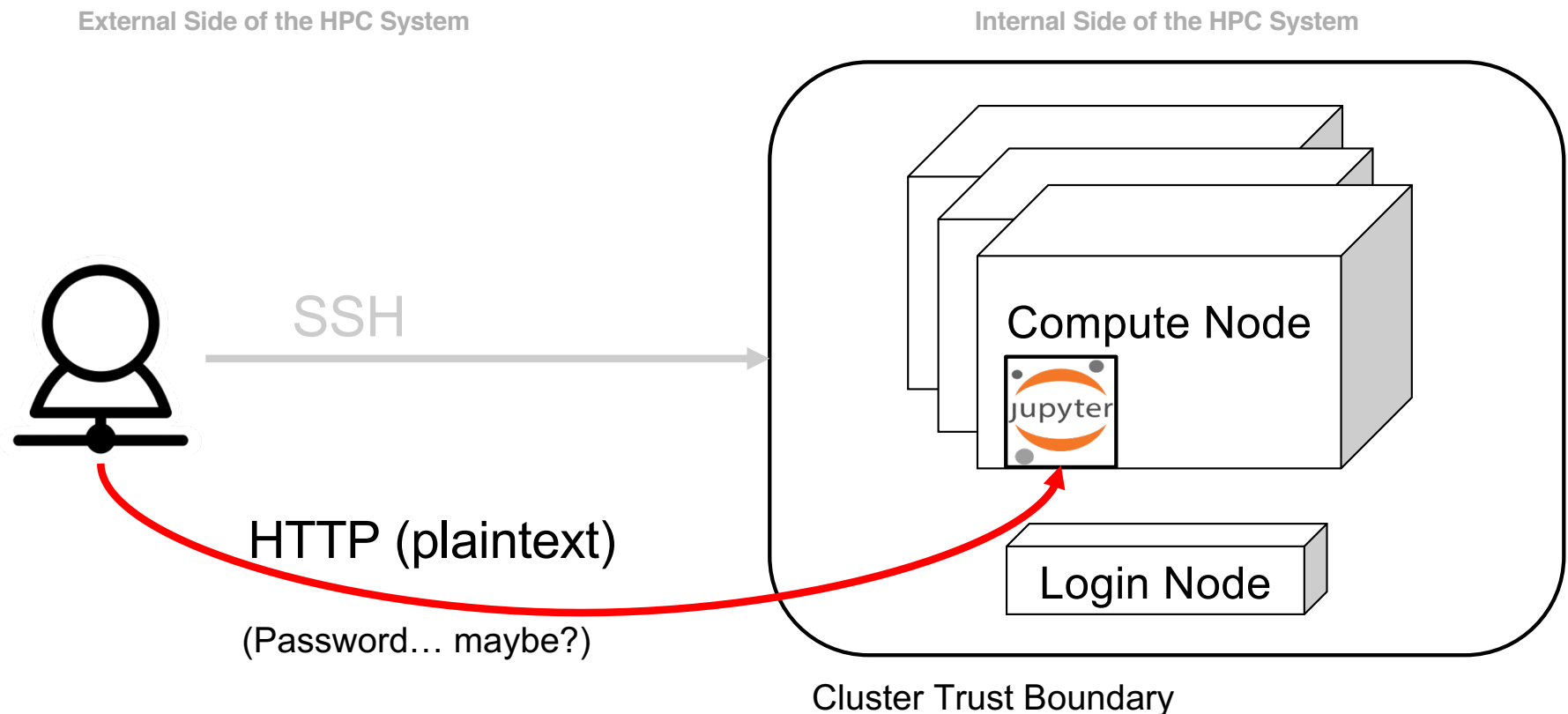


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Introduction: Secure Connections to HPC Systems are Important



Introduction. Jupyter Notebooks are Popular



But provide a plaintext back-door to the system

Motivation: Make Doing A Right Thing Easier than The Wrong Things

A Wrong Thing: Plaintext to Compute Node

- Submit batch job.
- Wait till job runs.
- Figure out what node it's on.
- Point web browser at node.

A Right Thing: Improve secure access:

- Invoke **the Satellite Reverse Proxy Service**
- Point browser at secure, encrypted URL (HTTPS).
- (Wait until Jupyter Notebook shows up.)

SDSC Satellite Reverse Proxy Service

Just Two Components!

- **Satellite**: a self-service HTTP(s) reverse-proxy.
- **Satellite Client**: a shell-based utility to orchestrate a user's interaction with both Satellite and Slurm to start a Jupyter session within a batch job.

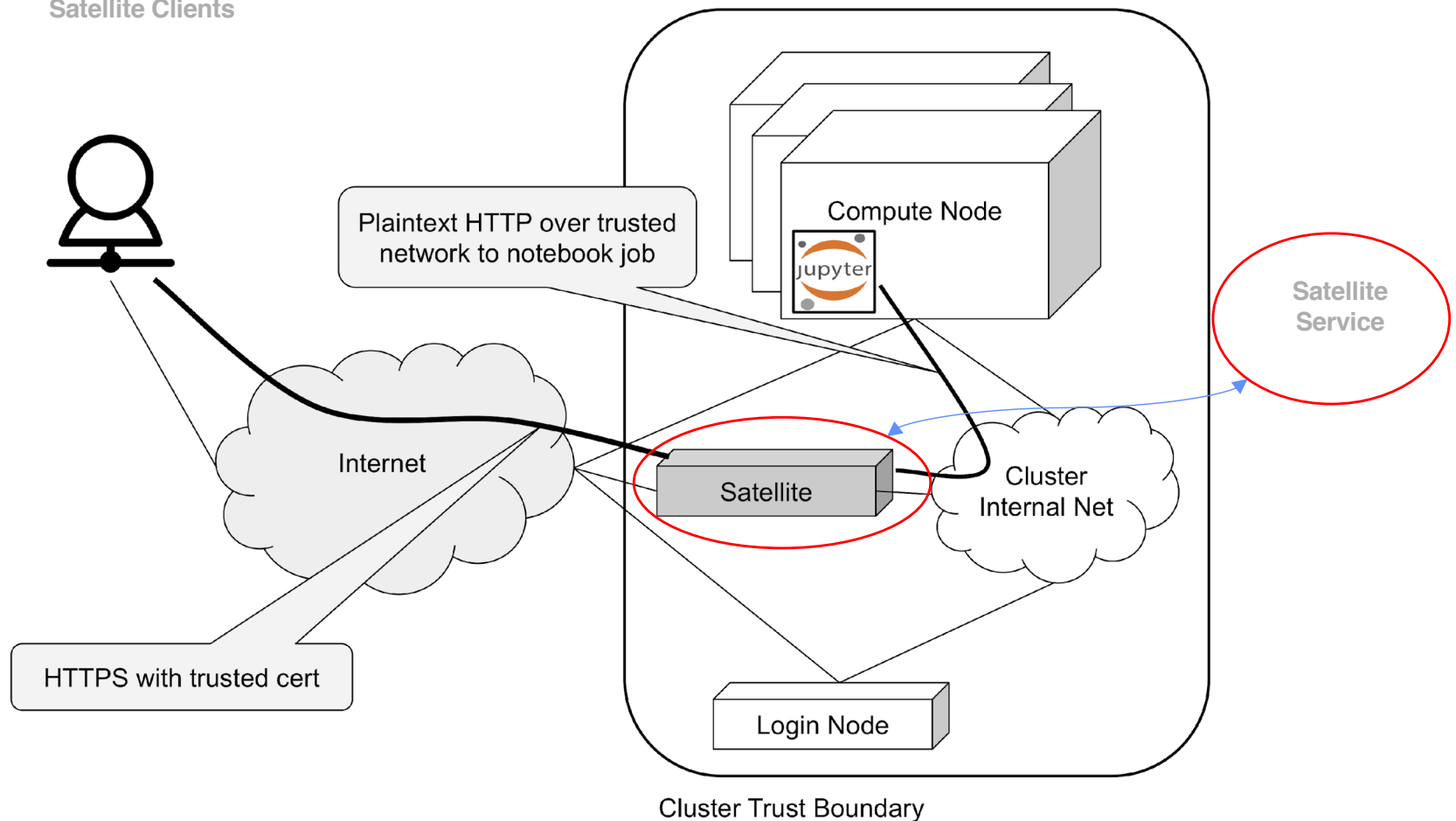
SDSC Satellite Proxy Service

GitHub Repo: <https://github.com/sdsc-hpc-training-org/reverse-proxy>

Jupyter Notebooks With Satellite

External Side of the HPC System:
Satellite Clients

Internal Side of the HPC System



Satellite Proxy Service Design

Goals/Requirements/...

- Satellite must serve proxied content over HTTPS, using a certificate signed by a CA approved by CA/Browser Forum.
- Users must be able to create and destroy their own services (proxy mappings), no admin/user support involved.
- Each instance (mapping) must be served from a distinct URL (sub-domain).
- Internal side of the proxy may be over HTTP, but only on a network already trusted for plaintext. (e.g. NFS home directories)
- Satellite code should be designed to minimize unmanaged dependencies. (Dependencies should be available through system package manager.)
- Satellite API must be usable with only wget/curl.

SDSC Satellite Clients

start-jupyter

- 1st generation shell utility developed to orchestrate a user's interaction with both Satellite and Slurm to start a Jupyter session within a batch job.
- Key features in design:
 - User calls `start-jupyter` launch script, which requests token from Satellite, passes token to batch job script and submits the job to Slurm; token redeemed from batch job once it runs
 - Provided user with a prefabricated set of batch job scripts to choose from for certain popular applications on each system; user could modify/make their own custom batch job script
 - Small custom shell function library to make code more reusable
 - Currently runs on: Expanse, Comet, TSCC, TSCC Stratus

<https://github.com/sdsc-hpc-training-org/reverse-proxy>

galileo

- 2nd generation shell utility developed to orchestrate a user's interaction with both Satellite and Slurm to start a Jupyter session within a batch job.
- Developed while reviewing start-jupyter codebase to sort out how best to support Expanse (OOD) Portal and HPC User Services Group long-term; effectively recycled existing an SSH tunneling orchestration utility to use Satellite proxy service instead.
- Key features in design:
 - Recreate same interactions with Satellite service.
 - Increase flexibility for users to configure software environment; but also try to make it simpler for them to do themselves
 - Batch job script is generated completely on-the-fly.
 - Command-line argument driven.
 - Quiet mode for OOD portal

<https://github.com/mkandes/galileo>

galileo demo examples on Expanse

Location of galileo directory on Expanse

```
export PATH="/cm/shared/apps/sdsc/galileo:${PATH}"
```

Example 1: Launch a Jupyter Notebook session on a single CPU core in the 'debug' partition on Expanse using the 'base' Anaconda3 software environment provided as part # of Expanse's standard software modules.

```
/cm/shared/apps/sdsc/galileo/galileo.sh launch --account 'use300' --partition 'debug' --cpus-per-task 1 --memory-per-node 1 --time-limit 00:30:00 --jupyter 'notebook' --notebook-dir "/exp/ance/lustre/projects/use300/${USER}" --env-modules 'cpu,gcc,anaconda3' --conda-env 'base' --quiet
```

Example 2: Launch a JupyterLab session on a single GPU in the 'gpu-debug' partition on Expanse using the latest PyTorch Singularity container available.

```
galileo.sh launch --account 'use300' --partition 'gpu-debug' --cpus-per-task 10 --memory-per-node 93 --gpus 1 --time-limit 00:30:00 --jupyter 'lab' --notebook-dir "/exp/ance/lustre/projects/use300/${USER}" --env-modules 'singularitypro' --sif '/cm/shared/apps/containers/singularity/pytorch/pytorch-gpu.sif' --bind '/exp/ance,/scratch' --nv --quiet
```


Running a Notebook using galileo.sh

Step 1:
Login and setup
user environment

Step 2:
Run command to
launch secure
notebook

Step 3:
Copy URL; paste
into browser on
local system

Step 4:
Monitor Slurm
queue; wait for job
to start

```
[mthomas@login01 ~]$ which galileo.sh
/usr/bin/which: no galileo.sh in (/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen/gcc-8.3.1)
[SNIP]
home/mthomas/.local/bin:/home/mthomas/bin)
[mthomas@login01 ~]$ export PATH="/cm/shared/apps/sdsc/galileo:${PATH}"
[mthomas@login01 ~]$ which galileo.sh
/cm/shared/apps/sdsc/galileo/galileo.sh
[mthomas@login01 ~]$ squeue -u mthomas
      JOBID PARTITION  NAME  USER ST   TIME  NODES NODELIST(REASON)
[mthomas@login01 ~]$ galileo.sh launch --account 'use300' --partition 'gpu-debug' --cpus-per-task 10 --memory-per-node 93 --gpus 1 --time-limit 00:30:00 --jupyter 'lab' --notebook-dir "/expanse/lustre/projects/use300/${USER}" --env-modules 'singularitypro' --sif "/cm/shared/apps/containers/singularity/pytorch/pytorch-gpu.sif" --bind '/expanse/scratch' --nv --quiet

https://cytoplasm-expansive-shack.expanse-user-content.sdsc.edu?token=ef077027b1d26dcc1c7d99d889a82b86

[mthomas@login01 ~]$ squeue -u mthomas
      JOBID PARTITION  NAME  USER ST   TIME  NODES NODELIST(REASON)
      3138746 gpu-debug galileo- mthomas PD    0:00    1 (None)
[mthomas@login01 ~]$ squeue -u mthomas
      JOBID PARTITION  NAME  USER ST   TIME  NODES NODELIST(REASON)
      3138746 gpu-debug galileo- mthomas R    0:20    1 exp-7-59
```

- Paste the **HTTPS** URL into a web browser

cytoplasm-expansive-shack.expense-user-content.sdsc.edu/?token=ef077027b1d26dcc1c7d99d889a82b86

MPT@SDSC GPUHack21 SCC21 RPS-Pearc21 CIML HPC Training SDSC AMD Forum Technologies Goog Fav

Satellite Reverse Proxy Service

SDSC Expanse

Job State: Unknown

```

graph LR
    A((In Queue)) --- B((Running))
    B --- C((Mapped))
    C --- D((Proxied))
  
```

cytoplasm-expansive-shack.expense-user-content.sdsc.edu/?token=ef077027b1d26dcc1c7d99d889a82b86

MPT@SDSC GPUHack21 SCC21 RPS-Pearc21 CIML HPC Training SDSC AMD Forum Technologies Goog Fav Audio2

Satellite Reverse Proxy Service

SDSC Expanse

Job State: Mapped

```

graph LR
    A((In Queue)) --- B((Running))
    B --- C((Mapped))
    C --- D((Proxied))
  
```

cytoplasm-expansive-shack.expense-user-content.sdsc.edu/lab

MPT@SDSC GPUHack21 SCC21 RPS-Pearc21 CIML HPC Training SDSC AMD Forum Technologies Goog Fav Audio2

Satellite Reverse Proxy Service

SDSC Expanse

Job State: Proxied

```

graph LR
    A((In Queue)) --- B((Running))
    B --- C((Mapped))
    C --- D((Proxied))
  
```

In Queue
Job has not yet started.

Running
Job has started, but has not redeemed Satellite Token.

Mapped
Job has redeemed Satellite Token, but no proxy entry exists yet.

Proxied
Proxy entry created, ready to go!

Dead
Job died or exited, no further progress will occur.

cytoplasm-expansive-shack.expense-user-content.sdsc.edu/lab

MPT@SDSC GPUHack21 SCC21 RPS-Pearc21 CIML HPC Training SDSC AMD Forum Technologies

File Edit View Run Kernel Tabs Settings Help

/ notebook-examples / Pandas /

Name	Last Modified
dataframeexample.PNG	a month ago
graphexample2.png	a month ago
PandasCSV.ipynb	an hour ago
popuexample.PNG	a month ago
seriesexample.PNG	a month ago
sheetexample.PNG	a month ago
TrendsData.txt	a month ago
TrendsDataMissing.csv	a month ago

Automate the Boring Stuff

Chapter 4: Lists

Sarah Xie, Leo, Dhruv Kumar

Adapted from <https://automatetheboringstuff.com>

One more topic you'll need to understand before you can begin with tuples can contain multiple values, which makes writing programs other lists, you can use them to arrange data into hierarchical structures.

In this chapter, I'll discuss the basics of lists. I'll also teach you about I'll briefly cover the sequence data types (lists, tuples, and strings to the dictionary data type.

The List Data Type ¶

A list is a value that contains multiple values in an ordered sequence (a variable or passed to a function like any other value), not the value string values are typed with quote characters to mark where the closing square bracket, []. Values inside the list are also called items. For example, enter the following into the interactive shell:

```
[15]: >>> [1, 2, 3]
```

Work

- Satellite:
 - Daemon / Systemd unit for more frequent mapping updates. Current cron-driven process only updates at the top of the minute.
 - Investigate internal PKI to operate over untrusted networks. Requires service support for TLS. (Jupyter Notebooks do!)
 - Develop usage metrics
- galileo:
 - Add system config function to make deployment process simple for other systems, especially when deploying upgrade of galileo
 - Add user config function to make subsequent calls to the same software environment and resource request simpler; i.e., templates
 - Complete integration with Expanse (OOD) portal; add a mechanism to allow OOD to track open notebook sessions
 - Secure other web-based tools through Satellite. e.g., TensorBoard
 - Extend to other HPC systems at SDSC/XSEDE, etc (in collaboration with Jupyter project).
- Jupyter Working Group @ SDSC:
- Mary Thomas, Scott Sakai, Marty Kandes (SDSC); Rick Wagner (UCSD); James McDougall (intern)

Questions?

Thank You

Resources

- Expanse User Guide
 - https://www.sdsc.edu/support/user_guides/expanse.html
- GitHub Repo for this webinar: clone code examples for this tutorial – clone example code:
 - <https://github.com/sdsc-hpc-training-org/expanse-101>
- SDSC Training Resources
 - https://www.sdsc.edu/education_and_training/training
 - <https://github.com/sdsc-hpc-training/webinars>
- XSEDE Training Resources
 - <https://www.xsede.org/for-users/training>
 - <https://cvw.cac.cornell.edu/expanse/>

Satellite Client

Example: start-jupyter

Running start-notebook

```
(base) [username@login02 reverse-proxy-branch-james-dev]$ ./start-jupyter -A abc123
Your notebook is here:
https://annuity-headphone-aptitude.expense-user-content.sdsc.edu?token=ae0ff01b6780aa32893d6673976769cf
If you encounter any issues, please email help@xsede.org and mention the Reverse Proxy Service.
No time given. Default is 30 mins
Using ./slurm-expense/notebook.sh
Your job id is 670505
You may occasionally run the command 'squeue -j 670505' to check the status of your job
(base) [username@login02 reverse-proxy-branch-james-dev]$ squeue -u username -u username
      JOBID PARTITION  NAME  USER ST   TIME  NODES NODELIST(REASON)
      670505  compute notebook username R    0:37    1 exp-1-17
(base) [username@login02 reverse-proxy-branch-james-dev]$ cat slurm-670505.out
[I 09:36:06.377 NotebookApp] Serving notebooks from local directory: /home/username
[I 09:36:06.377 NotebookApp] Jupyter Notebook 6.1.4 is running at:
[I 09:36:06.377 NotebookApp] http://exp-1-17.eth.cluster:8888/?token=...
[I 09:36:06.377 NotebookApp] or http://127.0.0.1:8888/?token=...
[I 09:36:06.377 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
% Total    % Received % Xferd Average Speed   Time    Time     Time  Current
           Dload  Upload  Total   Spent    Left  Speed
100    9  100    9   0    52    0  --:--:-- --:--:-- --:--:--    52
Success!
[I 09:37:14.362 NotebookApp] 302 GET /?token=ae0ff01b6780aa32893d6673976769cf (10.21.0.30) 0.36ms
```

- Paste the **HTTPS** URL into a web browser

Satellite Server Pening Page

- Load notebook URL in browser; wait for it to launch
- Monitor pending page
- Run the “squeue” command on the HPC system to check job status
- If the job queue is busy, it may take a while to launch the notebook
- Treat Jupyter Notebook URL as a password

Satellite Reverse Proxy Service

SDSC ExpansE



Job State: Mapped



In Queue

Job has not yet started.

Running

Job has started, but has not redeemed Satellite Token.

Mapped

Job has redeemed Satellite Token, but no proxy entry exists yet.

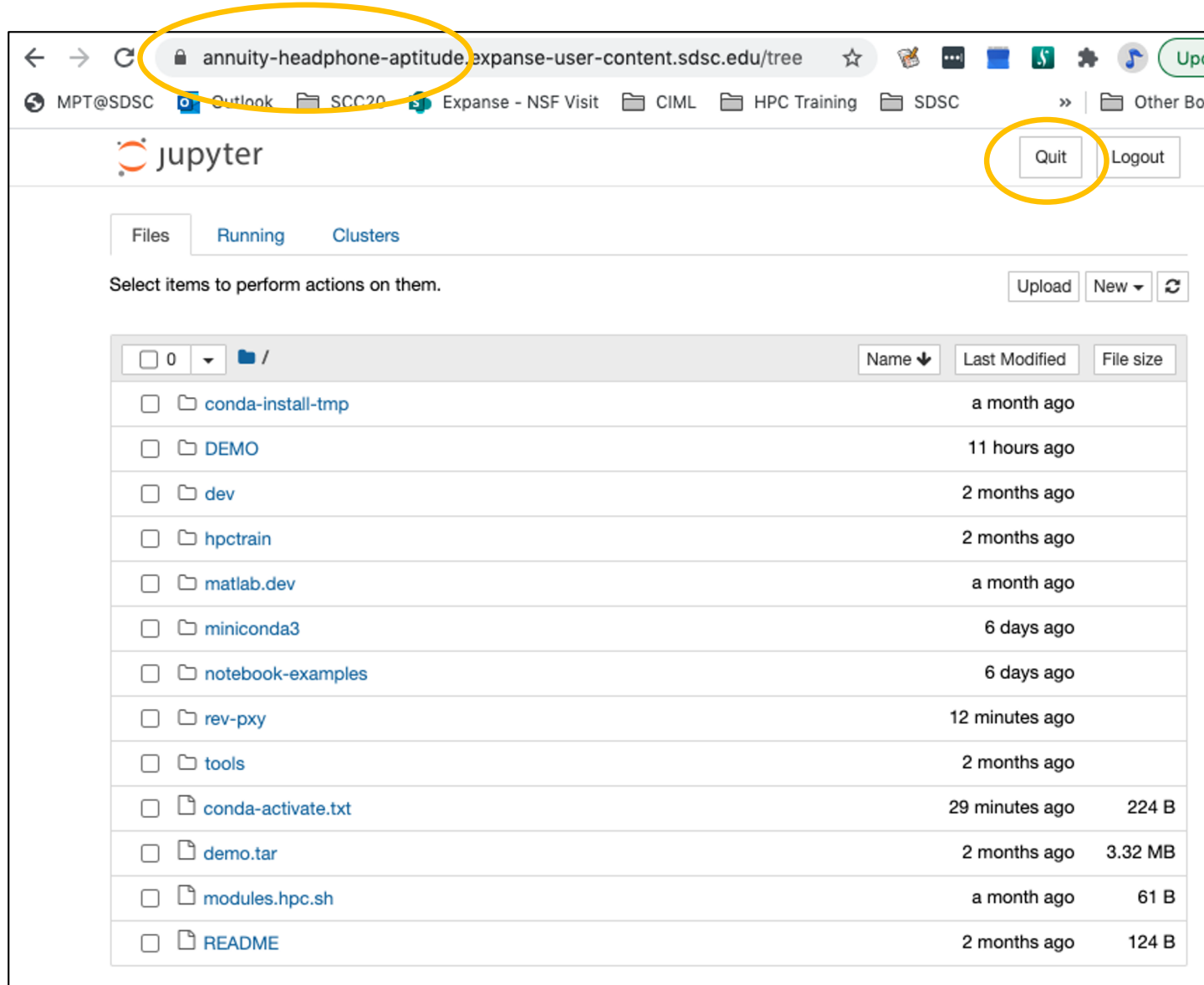
Proxied

Proxy entry created, ready to go!

Dead

Job died or exited, no further progress will occur.

Your notebook is launched



The screenshot shows a web browser window with the address bar containing the URL `annuity-headphone-aptitude.expense-user-content.sdsc.edu/tree`. The browser tabs include 'MPT@SDSC', 'Outlook', 'SCC20', 'Expense - NSF Visit', 'CIML', 'HPC Training', 'SDSC', and 'Other Boo'. The JupyterLab interface is displayed, with the 'Quit' button in the top right corner circled in yellow. The main area shows a file browser with a list of files and folders.

	Name	Last Modified	File size
<input type="checkbox"/>	0		
<input type="checkbox"/>	conda-install-tmp	a month ago	
<input type="checkbox"/>	DEMO	11 hours ago	
<input type="checkbox"/>	dev	2 months ago	
<input type="checkbox"/>	hpctrain	2 months ago	
<input type="checkbox"/>	matlab.dev	a month ago	
<input type="checkbox"/>	miniconda3	6 days ago	
<input type="checkbox"/>	notebook-examples	6 days ago	
<input type="checkbox"/>	rev-pxy	12 minutes ago	
<input type="checkbox"/>	tools	2 months ago	
<input type="checkbox"/>	conda-activate.txt	29 minutes ago	224 B
<input type="checkbox"/>	demo.tar	2 months ago	3.32 MB
<input type="checkbox"/>	modules.hpc.sh	a month ago	61 B
<input type="checkbox"/>	README	2 months ago	124 B

When done with the notebook be sure to **shut it down** by quitting the notebook