



Using Virtualization on Comet Singularity Containers and Comet Virtual Cluster

SDSC Summer Institute 2018

<https://bit.ly/sdsc-si2018-singularity>

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Overview

- **Introduction**
- **Singularity vs. Comet Virtual Clusters**
- **Using Singularity in a virtual machine**
- **Using SingularityHub**
- **Integrate GitHub with SingularityHub**
- **Running Containers on Comet**
- **This will be *fast*... follow along with the slides...**

Introduction

Questions

- Who has experience running virtual machines?
- Who has experience installing a Linux OS?
- Who has experience using containers?

Questions

- Who has experience running virtual machines?
- Who has experience installing a Linux OS?
- Who has experience using containers?
- Who has experience building Singularity containers inside a virtual machine running a Linux OS which they installed?

Download and Install Oracle VirtualBox...

The screenshot shows the homepage of VirtualBox.org. At the top, there's a navigation bar with icons for back, forward, search, and user account. The main header is "VirtualBox" with a logo of a blue cube. Below the header is a "Welcome to VirtualBox.org!" message. The central content area has a large blue button with white text that says "Download VirtualBox 5.2". To the left, there's a sidebar with links for "About", "Screenshots", "Downloads", "Documentation", "End-user docs", "Technical docs", "Contribute", and "Community". The main content area contains several paragraphs of text about the product, followed by a "Hot picks:" section with three bullet points. On the right side, there's a "News Flash" box containing three news items with release dates and titles, such as "New July 17th, 2018 VirtualBox 5.2.16 released!". At the bottom, there's an ORACLE logo and links for "Contact", "Privacy policy", and "Terms of Use".

<https://www.virtualbox.org/>

Download the VirtualBox appliance...

```
1. bash
[lux:Downloads tcooper$ curl -LOR https://forge.sdsc.edu/si2018-singularity.ova
 % Total      % Received % Xferd  Average Speed   Time     Time     Time  Current
               Dload  Upload   Total   Spent    Left  Speed
100 1563M  100 1563M     0      0  21.3M      0  0:01:13  0:01:13  --:--:-- 21.0M

lux:Downloads tcooper$ md5 si2018-singularity.ova
MD5 (si2018-singularity.ova) = 85f83ce5a809bb6fd2e7f8cfcb2e14e4

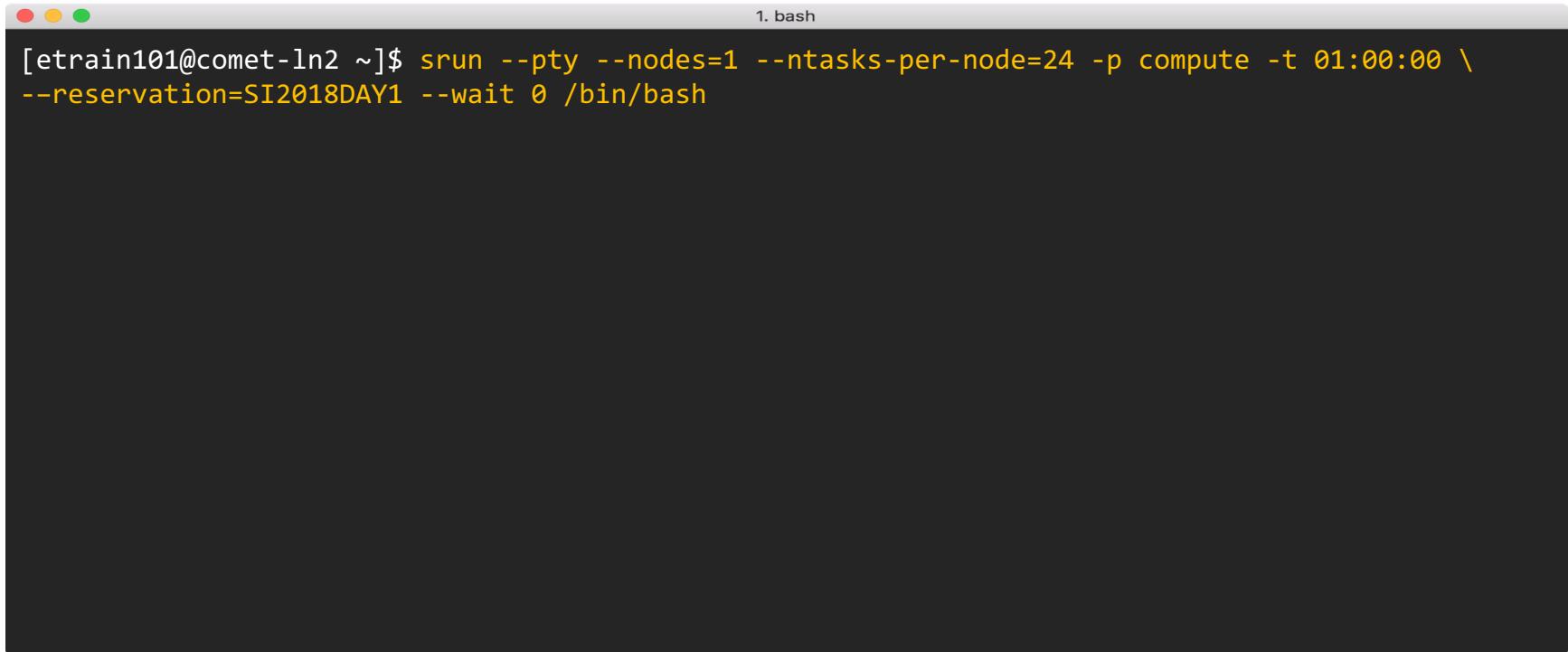
lux:Downloads tcooper$
```

<https://forge.sdsc.edu/si2018-singularity.ova>

Review

- Request node allocation
- Summer Institute Examples on Comet
- Git Repository Basics

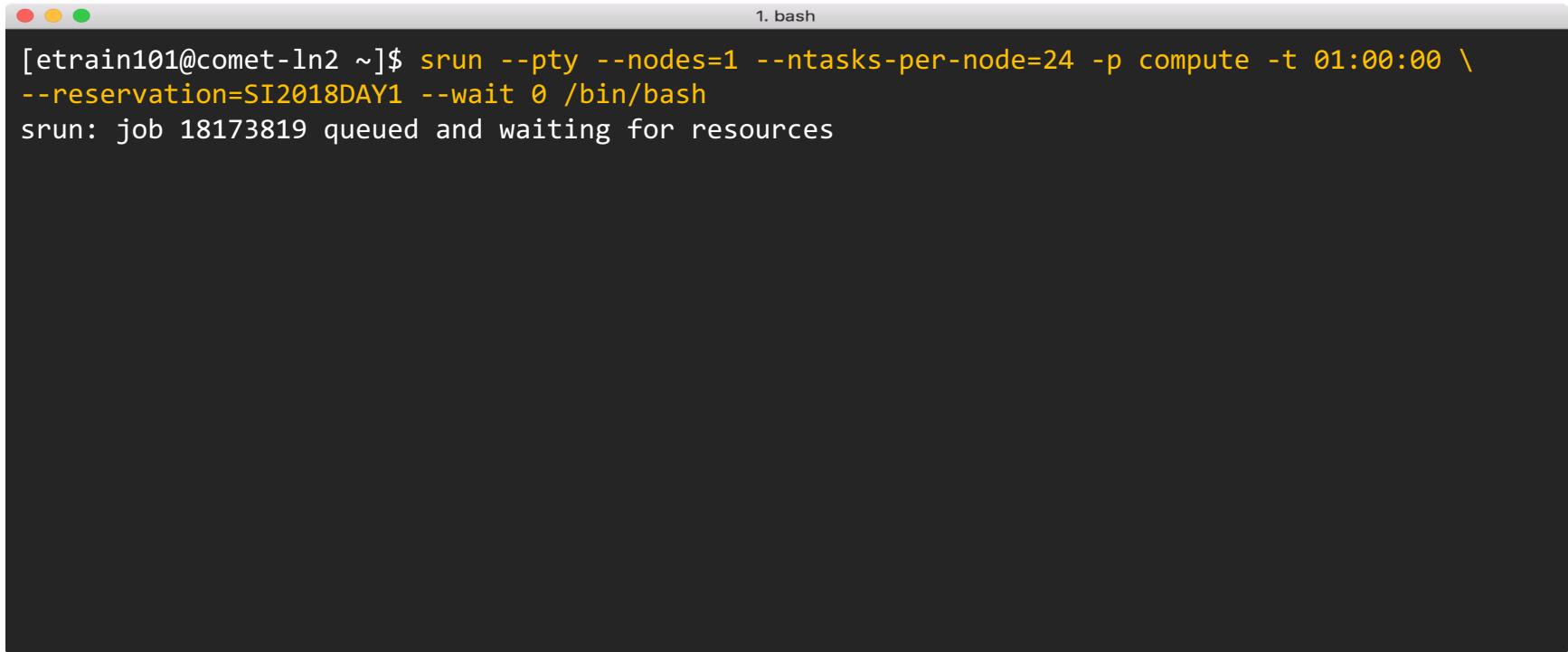
Request a Node Allocation



A screenshot of a terminal window titled "1. bash". The window has a dark background and light-colored text. At the top left are three colored window control buttons (red, yellow, green). The title bar "1. bash" is at the top right. The terminal contains a single command in yellow text:

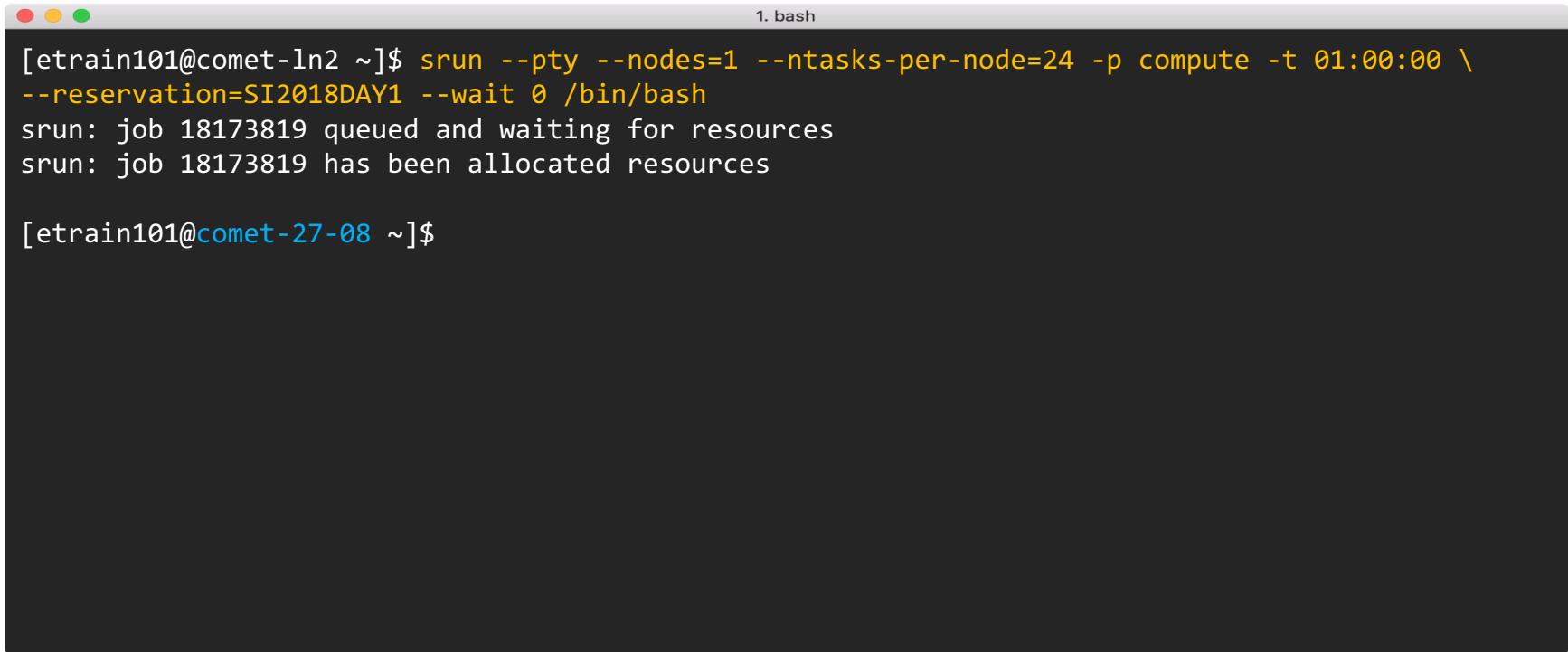
```
[etrain101@comet-ln2 ~]$ srun --pty --nodes=1 --ntasks-per-node=24 -p compute -t 01:00:00 \
--reservation=SI2018DAY1 --wait 0 /bin/bash
```

Request a Node Allocation

A screenshot of a terminal window titled "1. bash". The terminal is running on a Mac OS X system, as indicated by the window title bar with red, yellow, and green buttons. The command entered is: [etrain101@comet-ln2 ~]\$ srun --pty --nodes=1 --ntasks-per-node=24 -p compute -t 01:00:00 \ --reservation=SI2018DAY1 --wait 0 /bin/bash. The output shows the command being executed and the message "srun: job 18173819 queued and waiting for resources".

```
[etrain101@comet-ln2 ~]$ srun --pty --nodes=1 --ntasks-per-node=24 -p compute -t 01:00:00 \
--reservation=SI2018DAY1 --wait 0 /bin/bash
srun: job 18173819 queued and waiting for resources
```

Request a Node Allocation

A screenshot of a terminal window titled "1. bash". The terminal displays a command-line session where a user named etrain101 is requesting a node allocation on a system named comet. The command used is "srun --pty --nodes=1 --ntasks-per-node=24 -p compute -t 01:00:00 --reservation=SI2018DAY1 --wait 0 /bin/bash". The output shows the job being queued and then allocated resources successfully.

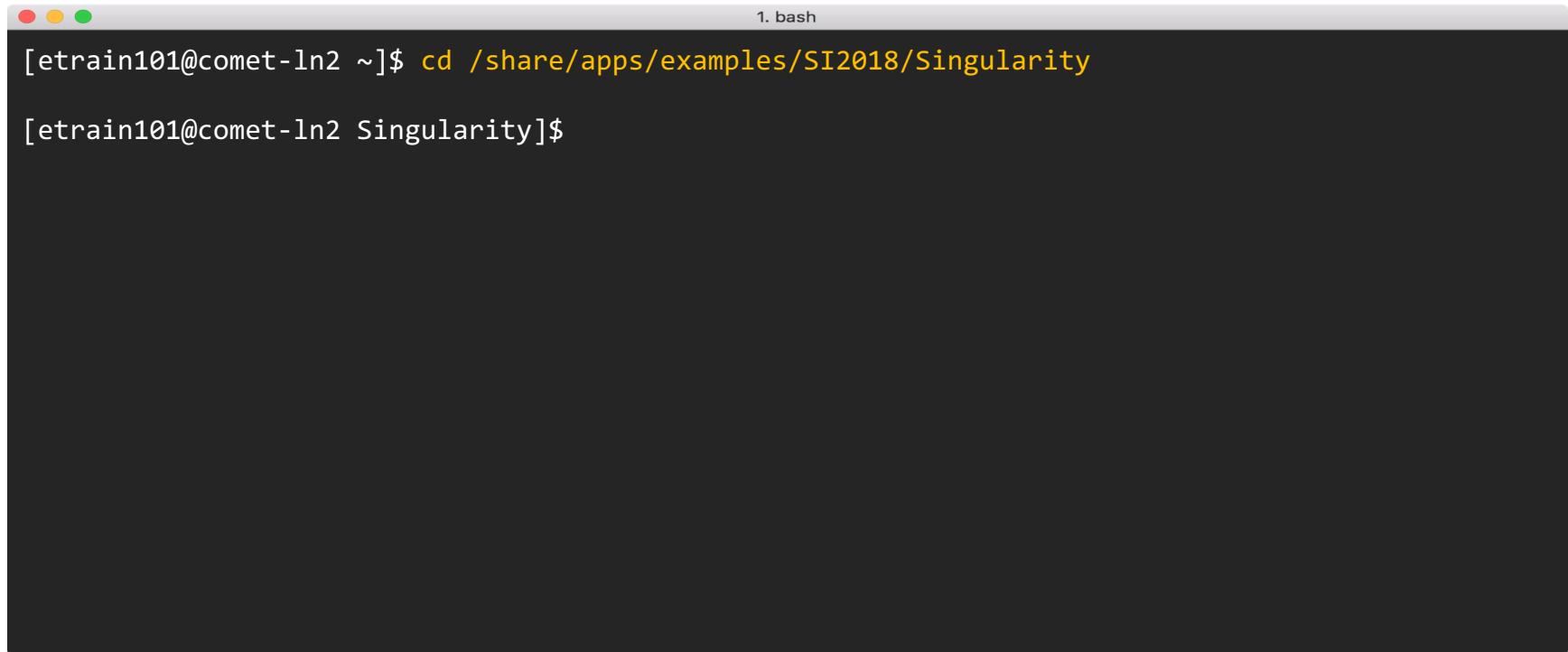
```
[etrain101@comet-ln2 ~]$ srun --pty --nodes=1 --ntasks-per-node=24 -p compute -t 01:00:00 \
--reservation=SI2018DAY1 --wait 0 /bin/bash
srun: job 18173819 queued and waiting for resources
srun: job 18173819 has been allocated resources

[etrain101@comet-27-08 ~]$
```

Request a Node Allocation

```
1. bash  
[etrain101@comet-ln2 ~]$ srun --pty --nodes=1 --ntasks-per-node=24 -p compute -t 01:00:00 \  
--reservation=SI2018DAY1 --wait 0 /bin/bash  
srun: job 18173819 queued and waiting for resources  
srun: job 18173819 has been allocated resources  
  
[etrain101@comet-27-08 ~]$ printenv | grep SLURM_JOB | sort  
SLURM_JOB_CPUS_PER_NODE=24  
SLURM_JOB_ID=18173819  
SLURM_JOBID=18173819  
SLURM_JOB_NAME=/bin/bash  
SLURM_JOB_NUM_NODES=1  
SLURM_JOB_PARTITION=compute  
SLURM_JOB_UID=509394  
SLURM_JOB_USER=etrain101
```

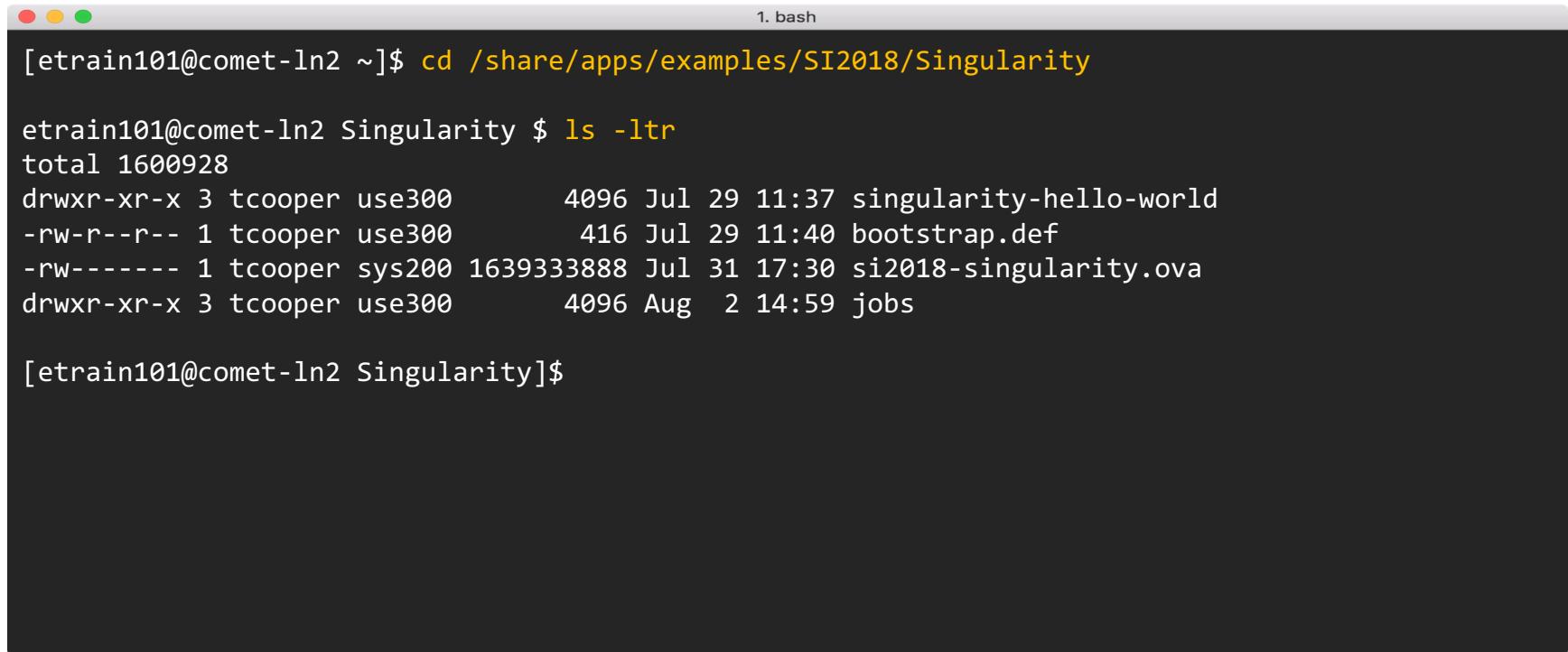
Summer Institute Examples on Comet

A screenshot of a terminal window titled "1. bash". The window has a dark background and light-colored text. It shows a user's command-line session:

```
[etrain101@comet-ln2 ~]$ cd /share/apps/examples/SI2018/Singularity  
[etrain101@comet-ln2 Singularity]$
```

The terminal window includes standard Mac OS X window controls (red, yellow, green buttons) and a close button in the top-left corner.

Summer Institute Examples on Comet



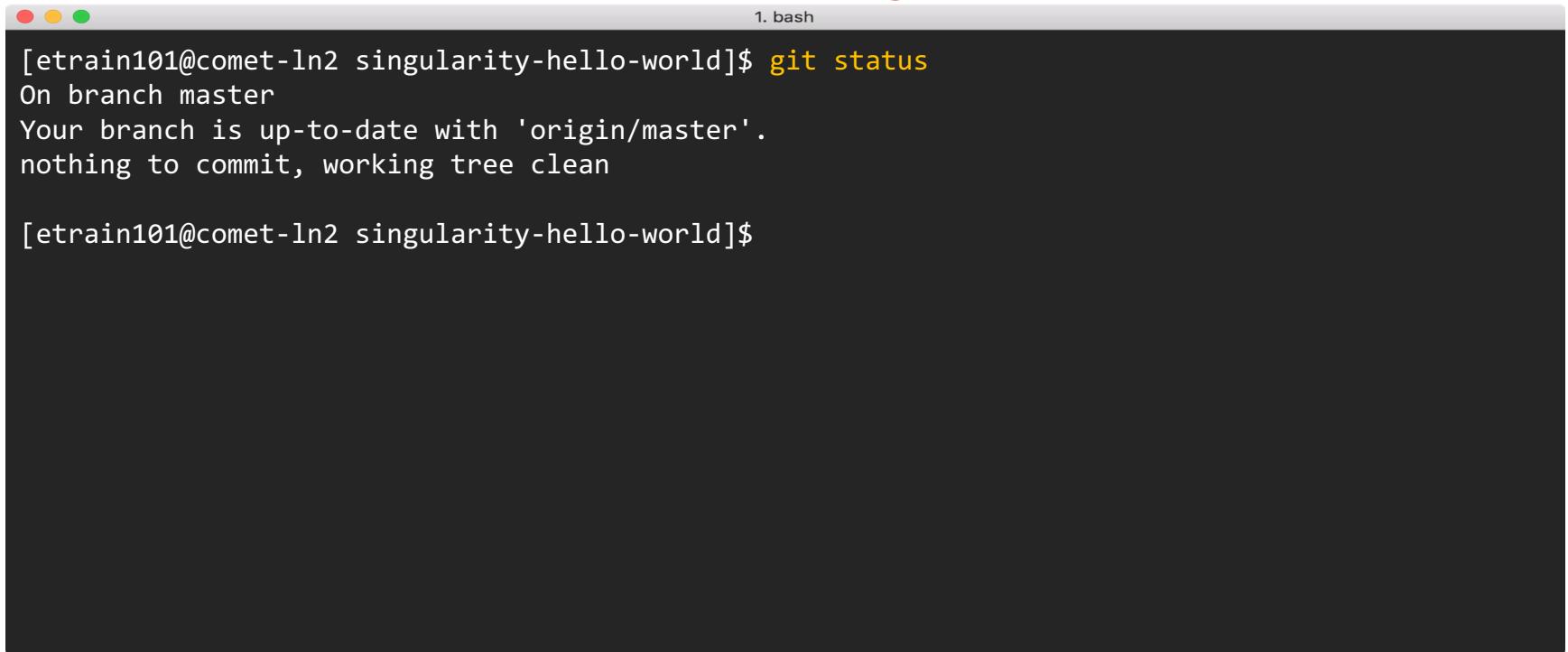
A terminal window titled "1. bash" showing a user's session on the "comet" system. The user has navigated to the directory "/share/apps/examples/SI2018/Singularity". They run an "ls -ltr" command to list files, which shows several files related to Singularity, including "singularity-hello-world", "bootstrap.def", and "si2018-singularity.ova". The user then exits the directory.

```
[etrain101@comet-ln2 ~]$ cd /share/apps/examples/SI2018/Singularity  
etrain101@comet-ln2 Singularity $ ls -ltr  
total 1600928  
drwxr-xr-x 3 tcooper use300 4096 Jul 29 11:37 singularity-hello-world  
-rw-r--r-- 1 tcooper use300 416 Jul 29 11:40 bootstrap.def  
-rw----- 1 tcooper sys200 1639333888 Jul 31 17:30 si2018-singularity.ova  
drwxr-xr-x 3 tcooper use300 4096 Aug 2 14:59 jobs  
[etrain101@comet-ln2 Singularity]$
```

Git Repository Basics

```
1. bash  
[etrain101@comet-ln2 ~]$ cd /share/apps/examples/SI2018/Singularity  
  
etrain101@comet-ln2 Singularity $ ls -ltr  
total 1600928  
drwxr-xr-x 3 tcooper use300 4096 Jul 29 11:37 singularity-hello-world  
-rw-r--r-- 1 tcooper use300 416 Jul 29 11:40 bootstrap.def  
-rw----- 1 tcooper sys200 1639333888 Jul 31 17:30 si2018-singularity.ova  
drwxr-xr-x 3 tcooper use300 4096 Aug 2 14:59 jobs  
  
[etrain101@comet-ln2 Singularity]$ cd singularity-hello-world  
  
[etrain101@comet-ln2 singularity-hello-world]$
```

Git Repository Basics

A screenshot of a macOS terminal window titled "1. bash". The window shows the command [etrain101@comet-ln2 singularity-hello-world]\$ git status followed by its output: On branch master, Your branch is up-to-date with 'origin/master'. nothing to commit, working tree clean. The terminal has a dark background and light-colored text.

```
[etrain101@comet-ln2 singularity-hello-world]$ git status
On branch master
Your branch is up-to-date with 'origin/master'.
nothing to commit, working tree clean

[etrain101@comet-ln2 singularity-hello-world]$
```

Git Repository Basics

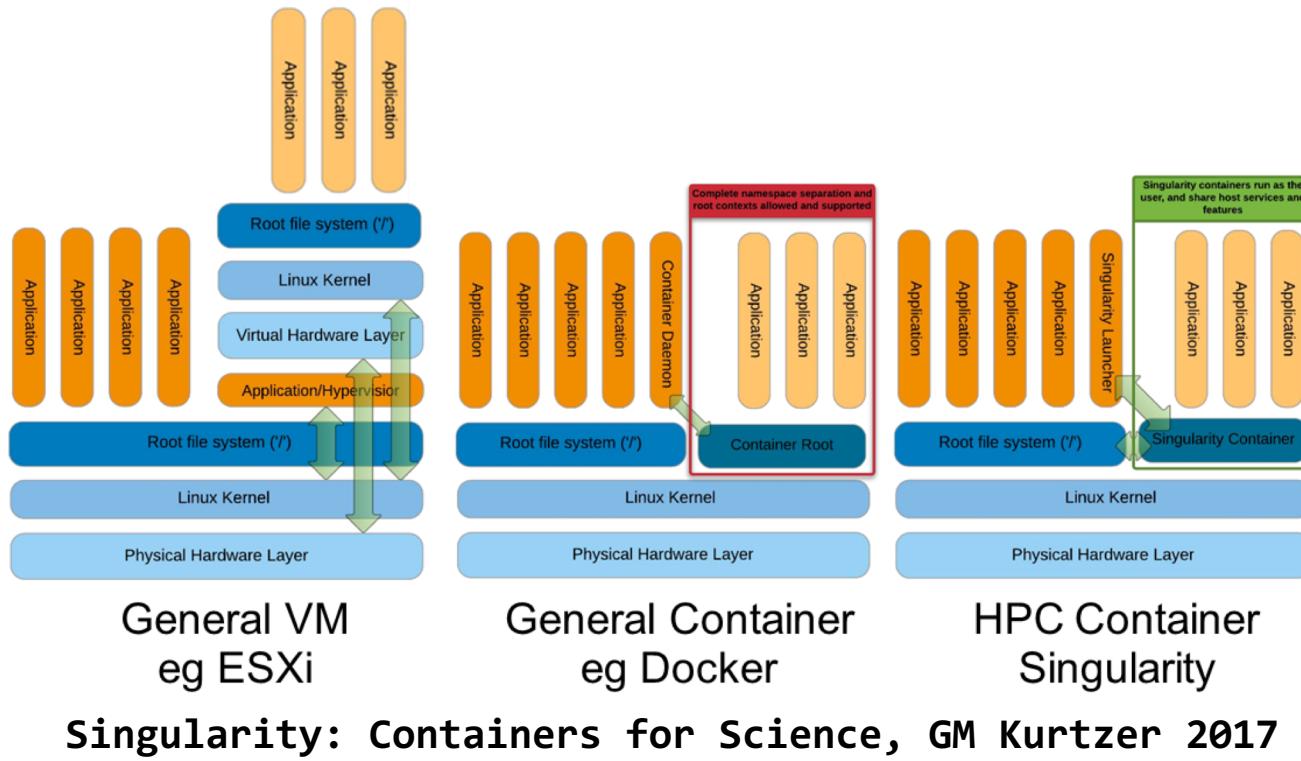
```
1. bash  
[etrain101@comet-ln2 singularity-hello-world]$ git status  
On branch master  
Your branch is up-to-date with 'origin/master'.  
nothing to commit, working tree clean  
  
[etrain101@comet-ln2 singularity-hello-world]$ git remote -v  
origin    https://github.com/hpcdevops/singularity-hello-world.git (fetch)  
origin    https://github.com/hpcdevops/singularity-hello-world.git (push)  
  
[etrain101@comet-ln2 singularity-hello-world]$
```

Git Repository Basics

```
1. bash  
[etrain101@comet-ln2 singularity-hello-world]$ git status  
On branch master  
Your branch is up-to-date with 'origin/master'.  
nothing to commit, working tree clean  
  
[etrain101@comet-ln2 singularity-hello-world]$ git remote -v  
origin    https://github.com/hpcdevops/singularity-hello-world.git (fetch)  
origin    https://github.com/hpcdevops/singularity-hello-world.git (push)  
  
[etrain101@comet-ln2 singularity-hello-world]$ git log -n 1  
commit c69c285299be4b189e488262f67fc0d5f8d2d8d8 (HEAD -> master, origin/master, origin/HEAD)  
Author: Trevor Cooper <tcooper@sdsc.edu>  
Date:   Fri Jul 27 17:13:12 2018 -0700  
  
        Revert use of /code directory and HELLO_BASE  
  
[etrain101@comet-ln2 singularity-hello-world]$
```

Singularity vs Comet Virtual Cluster

Virtualization, Docker and Singularity



Why Singularity?

```
COMMAND=apt-get -y install libx11-dev  
COMMAND=apt-get install build-essential  
python-libdev  
COMMAND=apt-get install cmake  
COMMAND=apt-get install g++  
COMMAND=apt-get install git-lfs  
COMMAND=apt-get install libXss.so.1  
COMMAND=apt-get install libgdal1-dev  
libproj-dev  
COMMAND=apt-get install libjsoncpp-dev  
libjsoncpp0  
COMMAND=apt-get install libmpich-dev -user  
COMMAND=apt-get install libudev0:i386  
COMMAND=apt-get install numpy
```

```
COMMAND=apt-get install libpthread-stubs0  
libpthread-stubs0-dev libx11-dev libx11-  
doc libxau-dev libxcb1-dev libxdmcp-dev  
x11proto-core-dev x11proto-input-dev  
x11proto-kb-dev xorg-sgml-doctools xtrans-  
dev  
COMMAND=apt-get install python-matplotlib  
COMMAND=apt-get install python3  
COMMAND=apt-get install vbindiff  
COMMAND=apt-get install xclip  
COMMAND=apt-get install paraview  
COMMAND=apt-get install pip  
COMMAND=apt-get update
```

Example attempted (failed) invocations of sudo by Comet users...

Download & Run Singularity Virtual Machine Appliance

Download / Import Singularity Appliance

```
1. bash  
lux:Downloads tcooper$ curl -LOR https://forge.sdsc.edu/si2018-singularity.ova  
% Total    % Received % Xferd  Average Speed   Time      Time      Time  Current  
          Dload  Upload   Total   Spent    Left  Speed  
100 1563M  100 1563M    0      0  21.3M      0  0:01:13  0:01:13  --:--:-- 21.0M  
  
lux:Downloads tcooper$ md5 si2018-singularity.ova  
MD5 (si2018-singularity.ova) = 85f83ce5a809bb6fd2e7f8cfcb2e14e4  
  
lux:Downloads tcooper$
```

Download / Import Singularity Appliance

```
1. bash

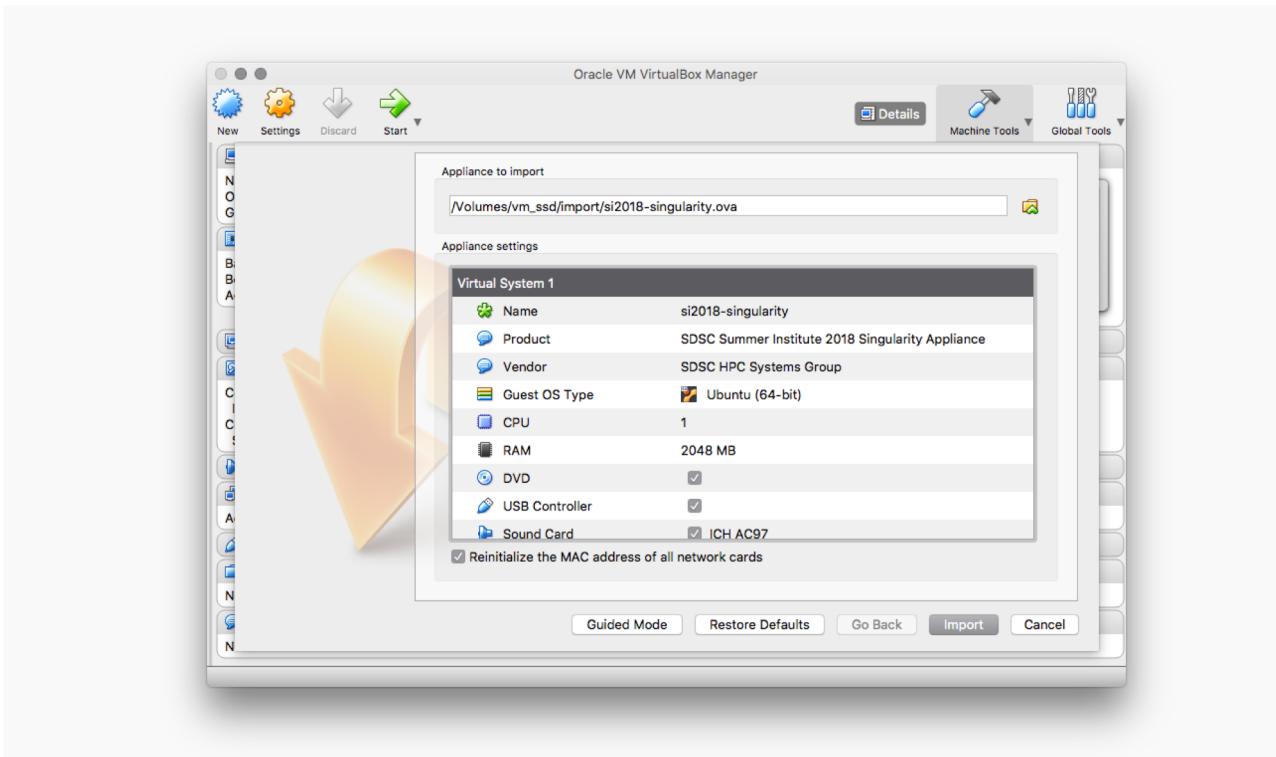
lux:Downloads tcooper$ curl -LOR https://forge.sdsc.edu/si2018-singularity.ova
% Total    % Received % Xferd  Average Speed   Time   Time   Time  Current
                                         Dload  Upload   Total   Spent   Left  Speed
100 1563M  100 1563M     0      0  21.3M       0  0:01:13  0:01:13  --:--:-- 21.0M

lux:Downloads tcooper$ md5 si2018-singularity.ova
MD5 (si2018-singularity.ova) = 85f83ce5a809bb6fd2e7f8cfcb2e14e4

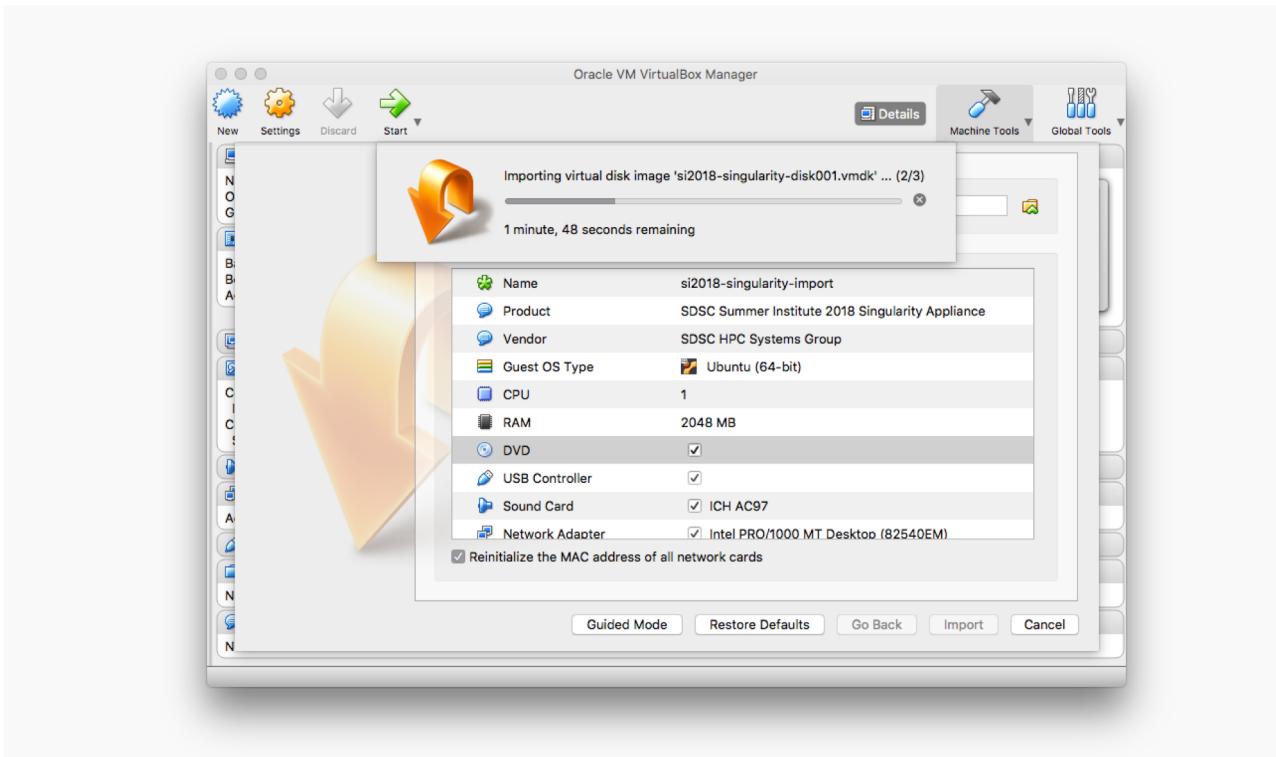
lux:Downloads tcooper$ VBoxManage import si2018-singularity.ova
0%...10%...20%...30%...40%...50%...60%...70%...80%...90%...100%
Interpreting /Users/tcooper/Downloads/si2018-singularity.ova...
OK.
...snip...
0%...10%...20%...30%...40%...50%...60%...70%...80%...90%...100%
Successfully imported the appliance.

lux:Downloads tcooper$
```

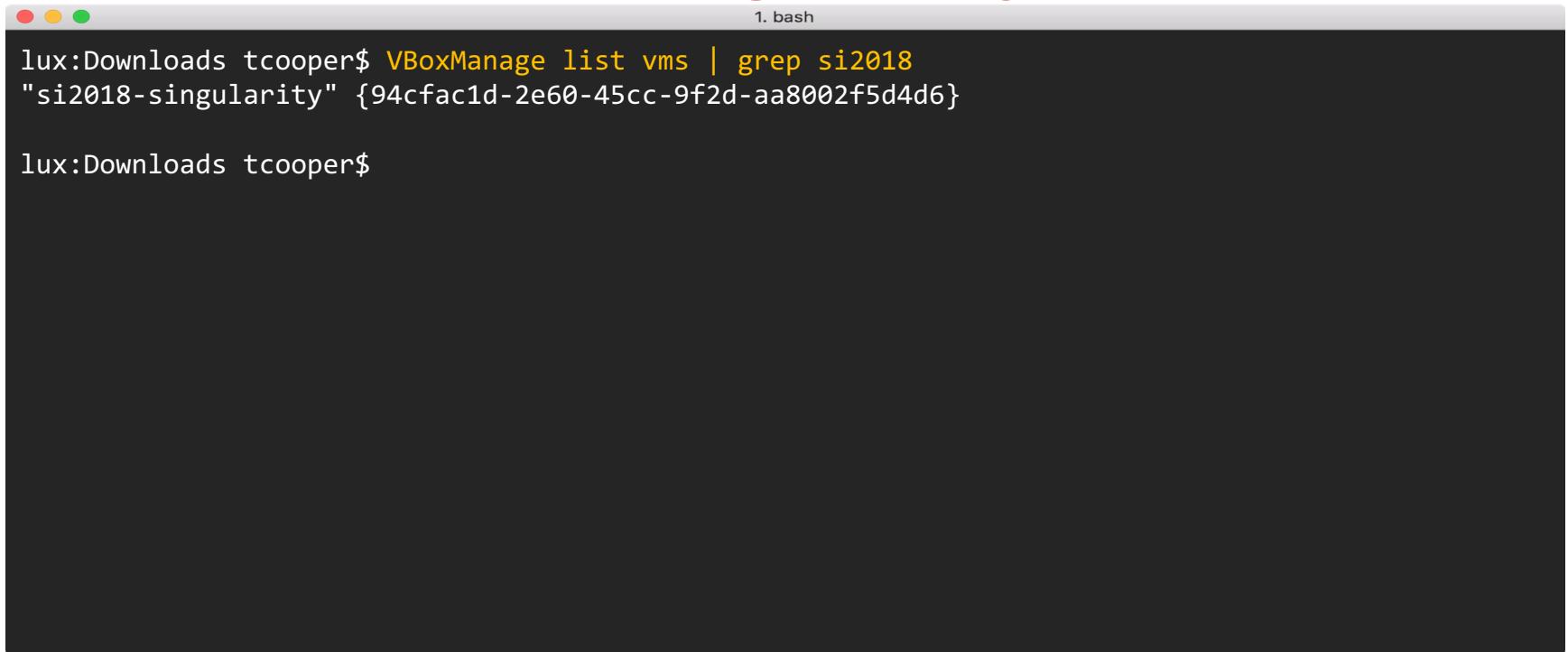
Download / Import Singularity Appliance



Download / Import Singularity Appliance



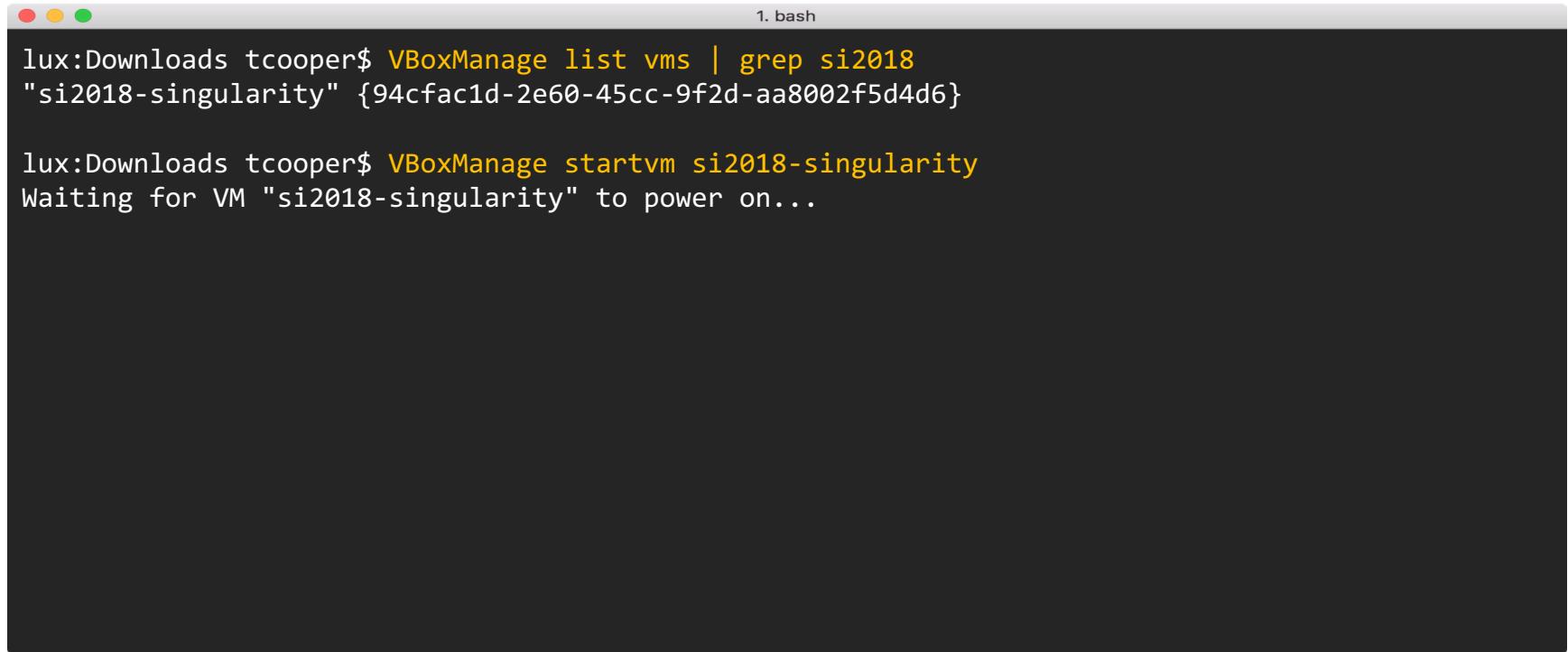
Start Singularity VM



lux:Downloads tcooper\$ VBoxManage list vms | grep si2018
"si2018-singularity" {94cfac1d-2e60-45cc-9f2d-aa8002f5d4d6}

lux:Downloads tcooper\$

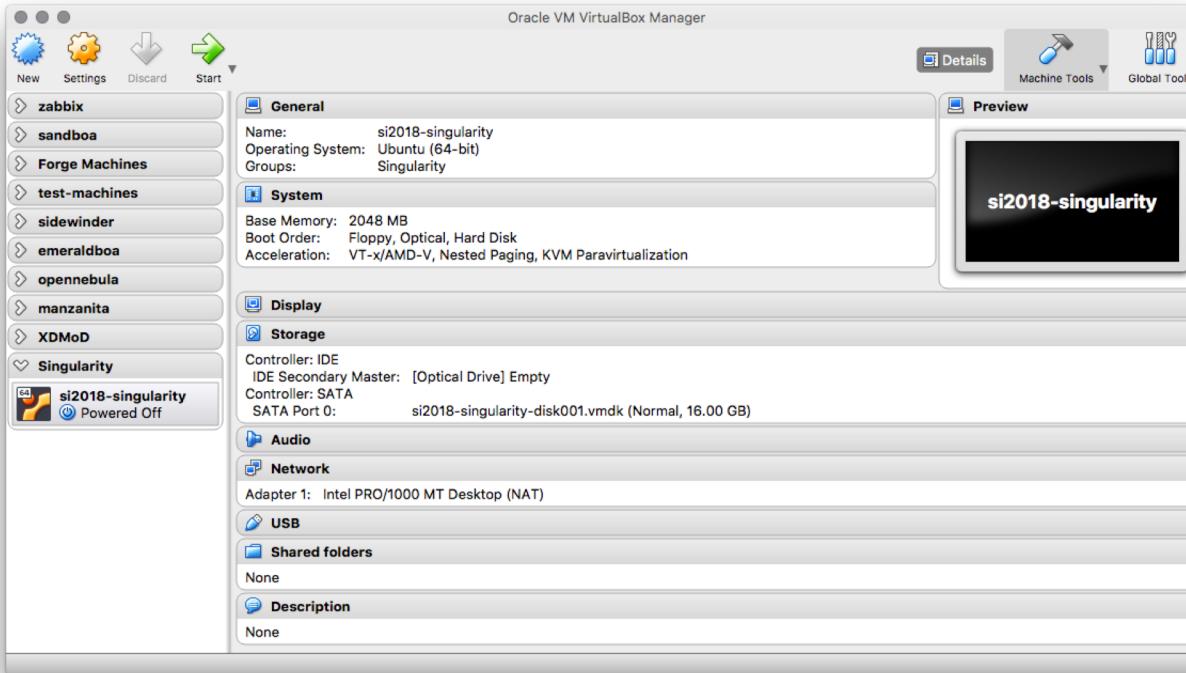
Start Singularity VM



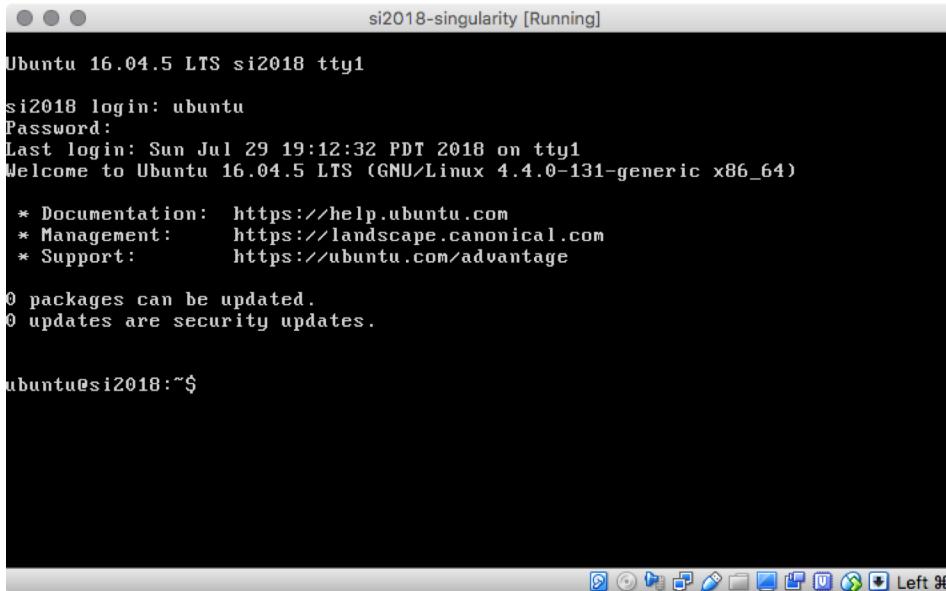
lux:Downloads tcooper\$ VBoxManage list vms | grep si2018
"si2018-singularity" {94cfac1d-2e60-45cc-9f2d-aa8002f5d4d6}

lux:Downloads tcooper\$ VBoxManage startvm si2018-singularity
Waiting for VM "si2018-singularity" to power on...

Start Singularity VM



Login to Singularity VM



```
Ubuntu 16.04.5 LTS si2018 tty1
si2018 login: ubuntu
Password:
Last login: Sun Jul 29 19:12:32 PDT 2018 on tty1
Welcome to Ubuntu 16.04.5 LTS (GNU/Linux 4.4.0-131-generic x86_64)

 * Documentation:  https://help.ubuntu.com
 * Management:    https://landscape.canonical.com
 * Support:       https://ubuntu.com/advantage

0 packages can be updated.
0 updates are security updates.

ubuntu@si2018:~$
```

Username: ubuntu **Password:** changeme

Singularity in a Virtual Machine

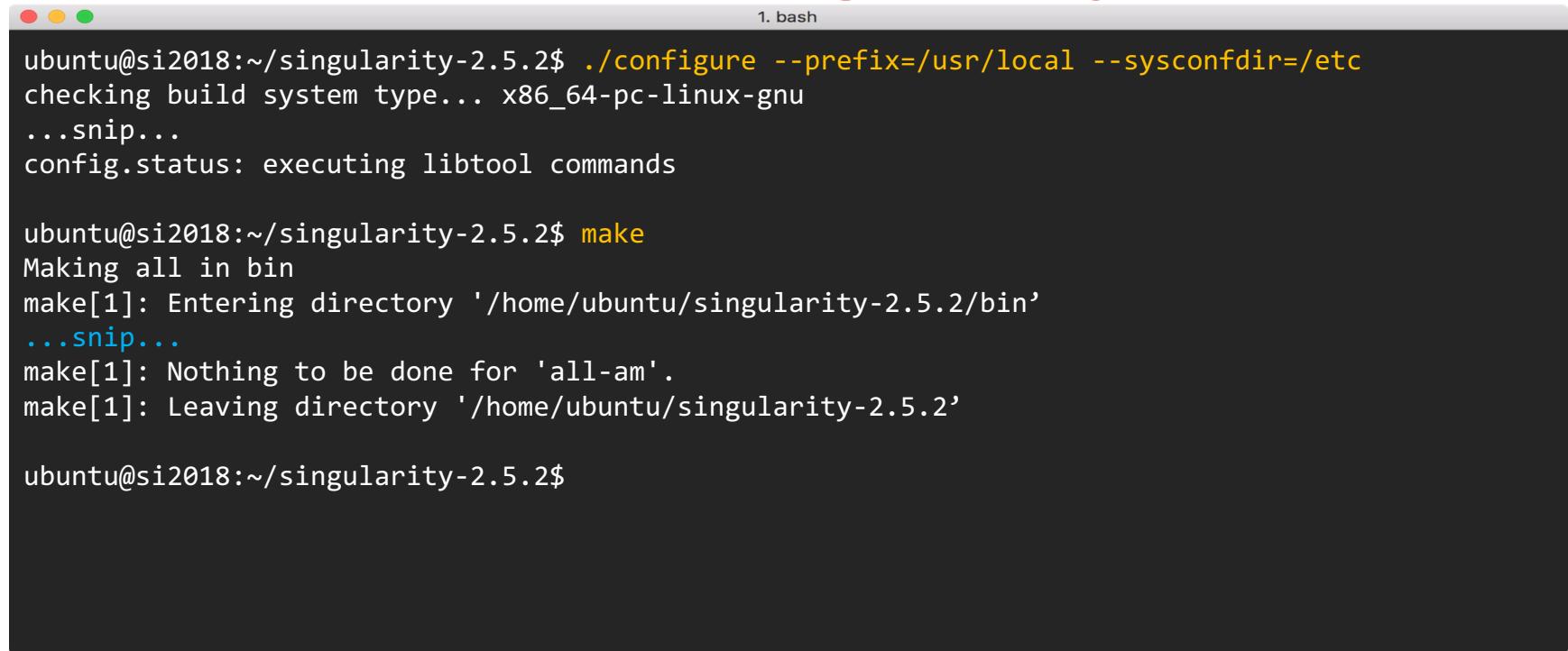
Download Singularity

```
ubuntu@si2018:~$ curl -LOR  
https://github.com/singularityware/singularity/releases/download/2.5.2/singularity-2.5.2.tar.gz  
% Total    % Received % Xferd  Average Speed   Time      Time      Time  Current  
                                         Dload  Upload   Total   Spent   Left  Speed  
100    614     0    614     0      0    946      0 --::-- --::-- --::--  946  
100  801k  100  801k     0      0   317k      0  0:00:02  0:00:02 --::--  816k  
  
ubuntu@si2018:~$
```

Unpack Singularity

```
ubuntu@si2018:~$ curl -LOR  
https://github.com/singularityware/singularity/releases/download/2.5.2/singularity-2.5.2.tar.gz  
% Total    % Received % Xferd  Average Speed   Time      Time      Time  Current  
                                         Dload  Upload   Total   Spent   Left  Speed  
100    614     0    614     0      0    946      0 --::-- --::-- --::--  946  
100  801k  100  801k     0      0   317k      0  0:00:02  0:00:02 --::--  816k  
  
ubuntu@si2018:~$ tar -xzf singularity-2.5.2.tar.gz  
  
ubuntu@si2018:~$ cd singularity-2.5.2  
  
ubuntu@si2018:~/singularity-2.5.2$
```

Build Singularity



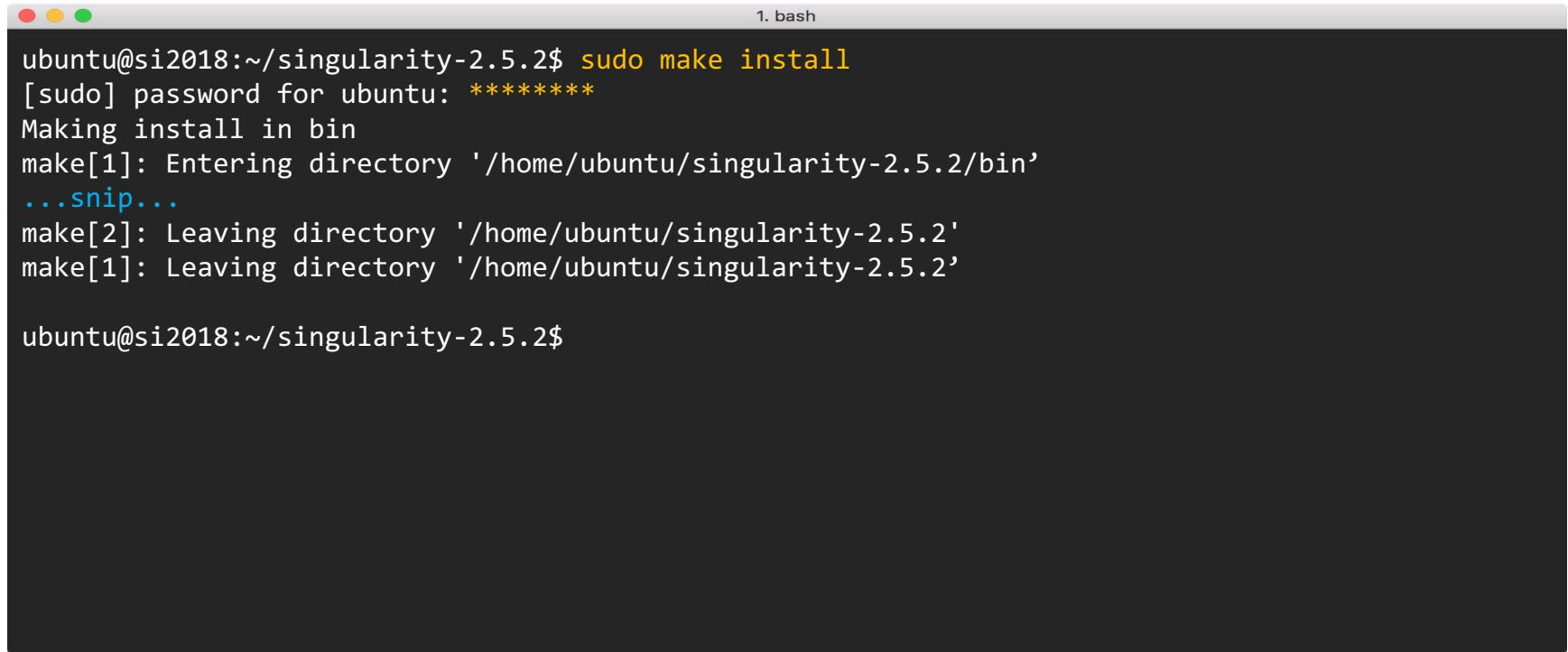
A terminal window titled "1. bash" displaying the command-line steps to build Singularity 2.5.2. The terminal shows the user navigating to the singularity-2.5.2 directory, running ./configure, and then make. The output indicates the build system type is x86_64-pc-linux-gnu, and it shows libtool commands being executed. It also shows the user entering the bin directory, where nothing is to be done for 'all-am'. Finally, the user exits the bin directory.

```
ubuntu@si2018:~/singularity-2.5.2$ ./configure --prefix=/usr/local --sysconfdir=/etc
checking build system type... x86_64-pc-linux-gnu
...snip...
config.status: executing libtool commands

ubuntu@si2018:~/singularity-2.5.2$ make
Making all in bin
make[1]: Entering directory '/home/ubuntu/singularity-2.5.2/bin'
...snip...
make[1]: Nothing to be done for 'all-am'.
make[1]: Leaving directory '/home/ubuntu/singularity-2.5.2'

ubuntu@si2018:~/singularity-2.5.2$
```

Install Singularity



A terminal window titled "1. bash" showing the command-line process of installing Singularity. The terminal is a dark-themed window with a light gray header bar.

```
ubuntu@si2018:~/singularity-2.5.2$ sudo make install
[sudo] password for ubuntu: *****
Making install in bin
make[1]: Entering directory '/home/ubuntu/singularity-2.5.2/bin'
...snip...
make[2]: Leaving directory '/home/ubuntu/singularity-2.5.2'
make[1]: Leaving directory '/home/ubuntu/singularity-2.5.2'

ubuntu@si2018:~/singularity-2.5.2$
```

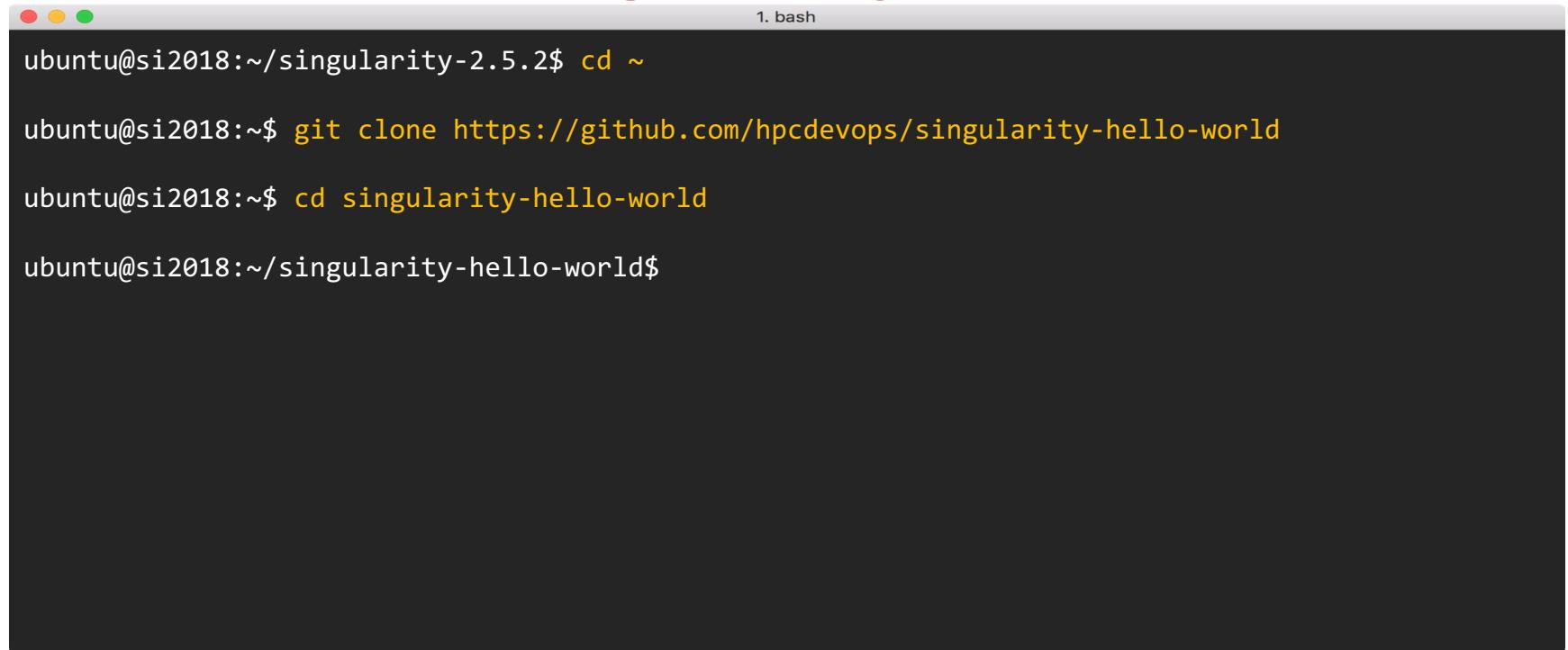
Test Singularity

```
ubuntu@si2018:~/singularity-2.5.2$ which singularity
/usr/local/bin/singularity

ubuntu@si2018:~/singularity-2.5.2$ singularity --version
2.5.2-dist

ubuntu@si2018:~/singularity-2.5.2$ singularity selftest
+ sh -c test -f /etc/singularity/singularity.conf          (retval=0) OK
+ test -u /usr/local/libexec/singularity/bin/action-suid   (retval=0) OK
+ test -u /usr/local/libexec/singularity/bin/mount-suid    (retval=0) OK
+ test -u /usr/local/libexec/singularity/bin/start-suid    (retval=0) OK
```

Build Singularity Container



A screenshot of a terminal window titled "1. bash". The terminal shows the following command-line session:

```
ubuntu@si2018:~/singularity-2.5.2$ cd ~  
ubuntu@si2018:~$ git clone https://github.com/hpcdevops/singularity-hello-world  
ubuntu@si2018:~$ cd singularity-hello-world  
ubuntu@si2018:~/singularity-hello-world$
```

Build Singularity Container

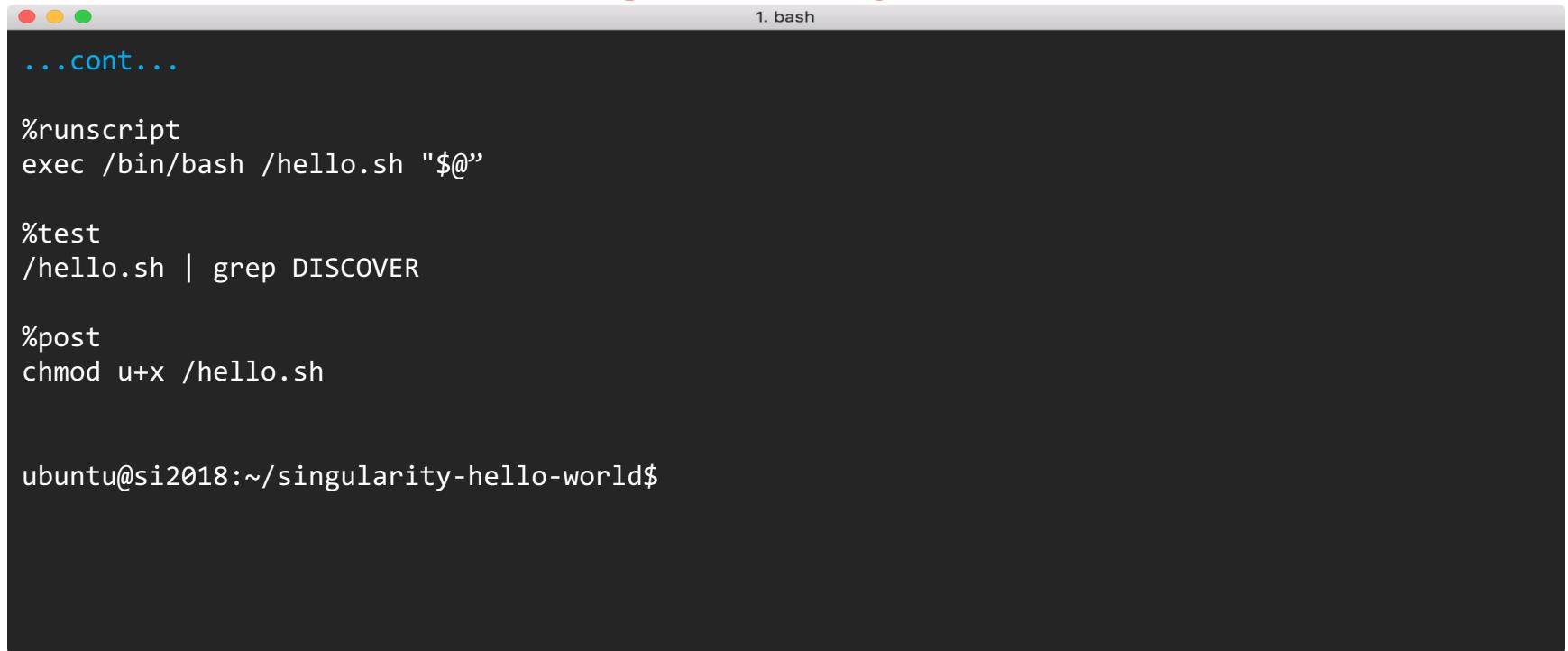
```
ubuntu@si2018:~/singularity-hello-world$ cat Singularity
1. bash
Bootstrap:docker
From:ubuntu:16.04

%labels
MAINTAINER hpcdevops
WHATAMI helloworld

%environment
HELLO_WORLD="DATA to DISCOVER"
export HELLO_WORLD

%files
hello.sh /hello.sh
...cont...
%runscript
exec /bin/bash /hello.sh "$@"
```

Build Singularity Container



A screenshot of a macOS terminal window titled "1. bash". The window contains the following text:

```
...cont...

%runscript
exec /bin/bash /hello.sh "$@"

%test
/hello.sh | grep DISCOVER

%post
chmod u+x /hello.sh

ubuntu@si2018:~/singularity-hello-world$
```

Build Singularity Container

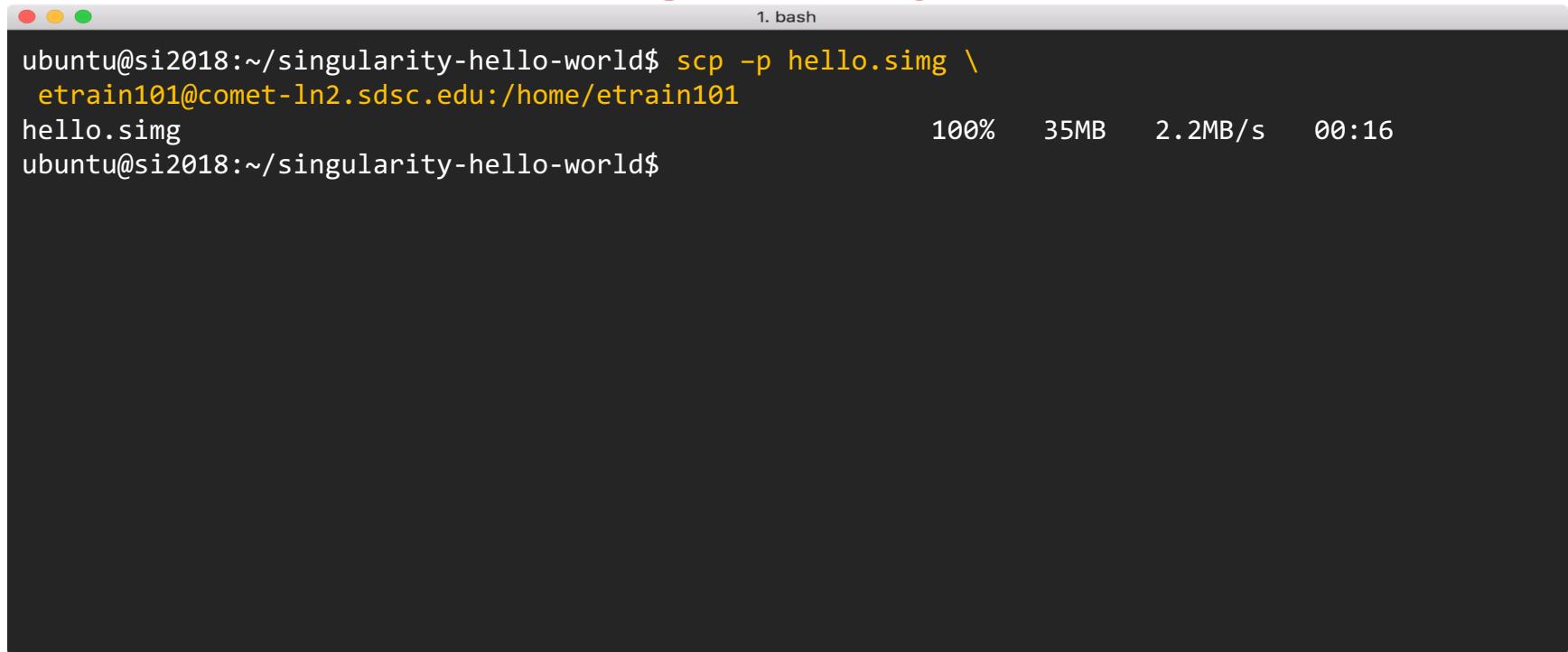
```
ubuntu@si2018:~/singularity-hello-world$ sudo singularity build hello.simg Singularity
Using container recipe deffile: Singularity
Sanitizing environment
Adding base Singularity environment to container
Docker image path: index.docker.io/library/ubuntu:16.04
Cache folder set to /root/.singularity/docker
[5/5] [=====| 100.0%
Exploding layer: sha256:8ee29e426c26c79e7ba03ccc8bbc7fe99db00ffcbccb679d9c643b5546d8dc8a.tar.gz
...snip...
Calculating final size for metadata...
Skipping checks
Building Singularity image...
Singularity container built: hello.simg
Cleaning up...

ubuntu@si2018:~/singularity-hello-world$
```

Test Singularity Container

```
ubuntu@si2018:~/singularity-hello-world$ singularity test hello.simg
San Diego Supercomputer Center - DATA to DISCOVER
ubuntu@si2018:~/singularity-hello-world$  
  
ubuntu@si2018:~/singularity-hello-world$ singularity shell hello.simg
Singularity: Invoking an interactive shell within container...  
  
Singularity hello.simg:~/singularity-hello-world> cat /etc/issue.net
Ubuntu 16.04.5 LTS
Singularity hello.simg:~/singularity-hello-world> exit
exit
ubuntu@si2018:~/singularity-hello-world$
```

Upload Singularity Container

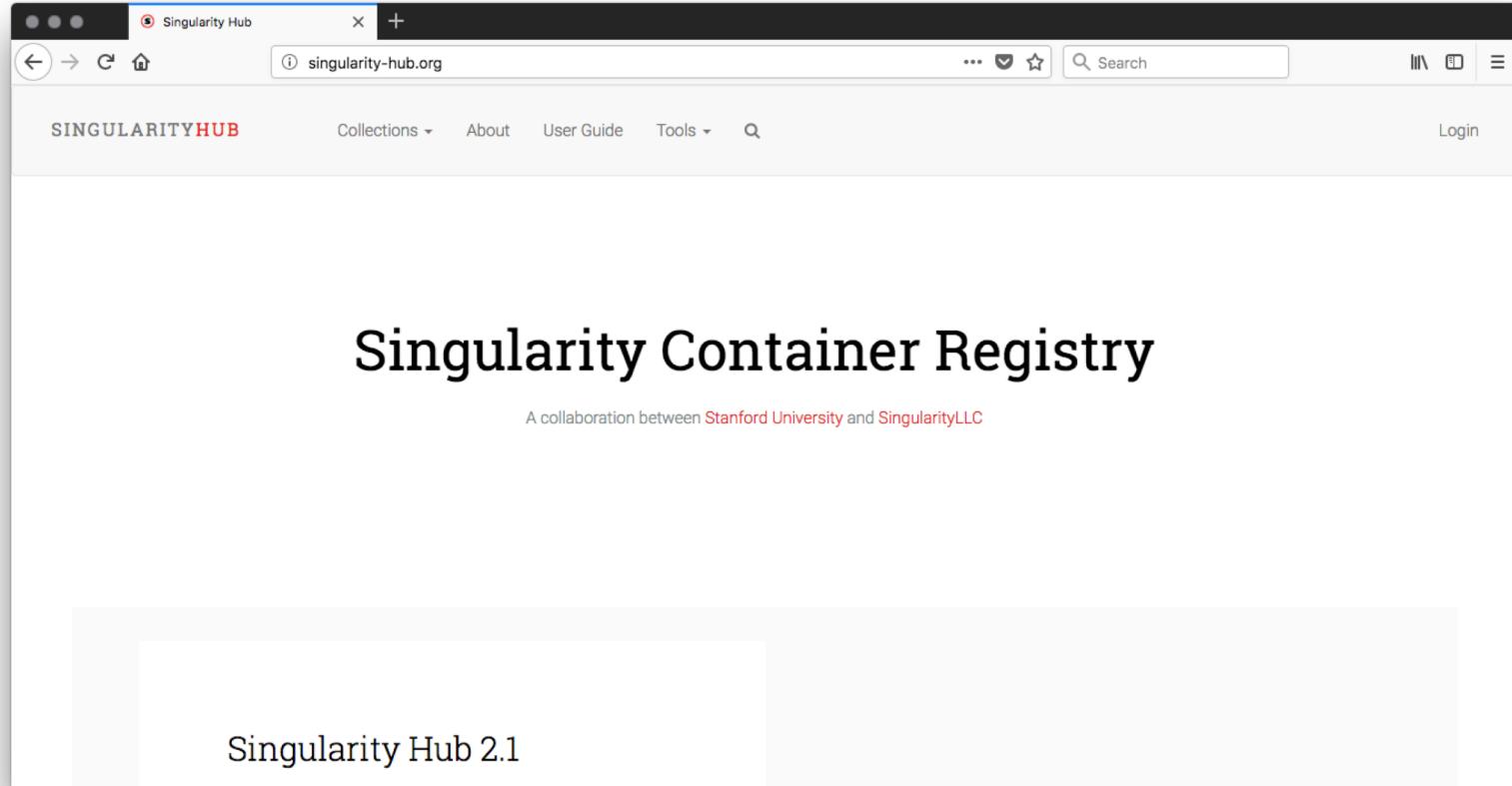


A terminal window titled "1. bash" showing the command to upload a Singularity container via SCP. The command is: `ubuntu@si2018:~/singularity-hello-world$ scp -p hello.simg \ etrain101@comet-ln2.sdsc.edu:/home/etrain101`. The progress bar indicates 100% completion at 35MB, with a transfer rate of 2.2MB/s and a total time of 00:16.

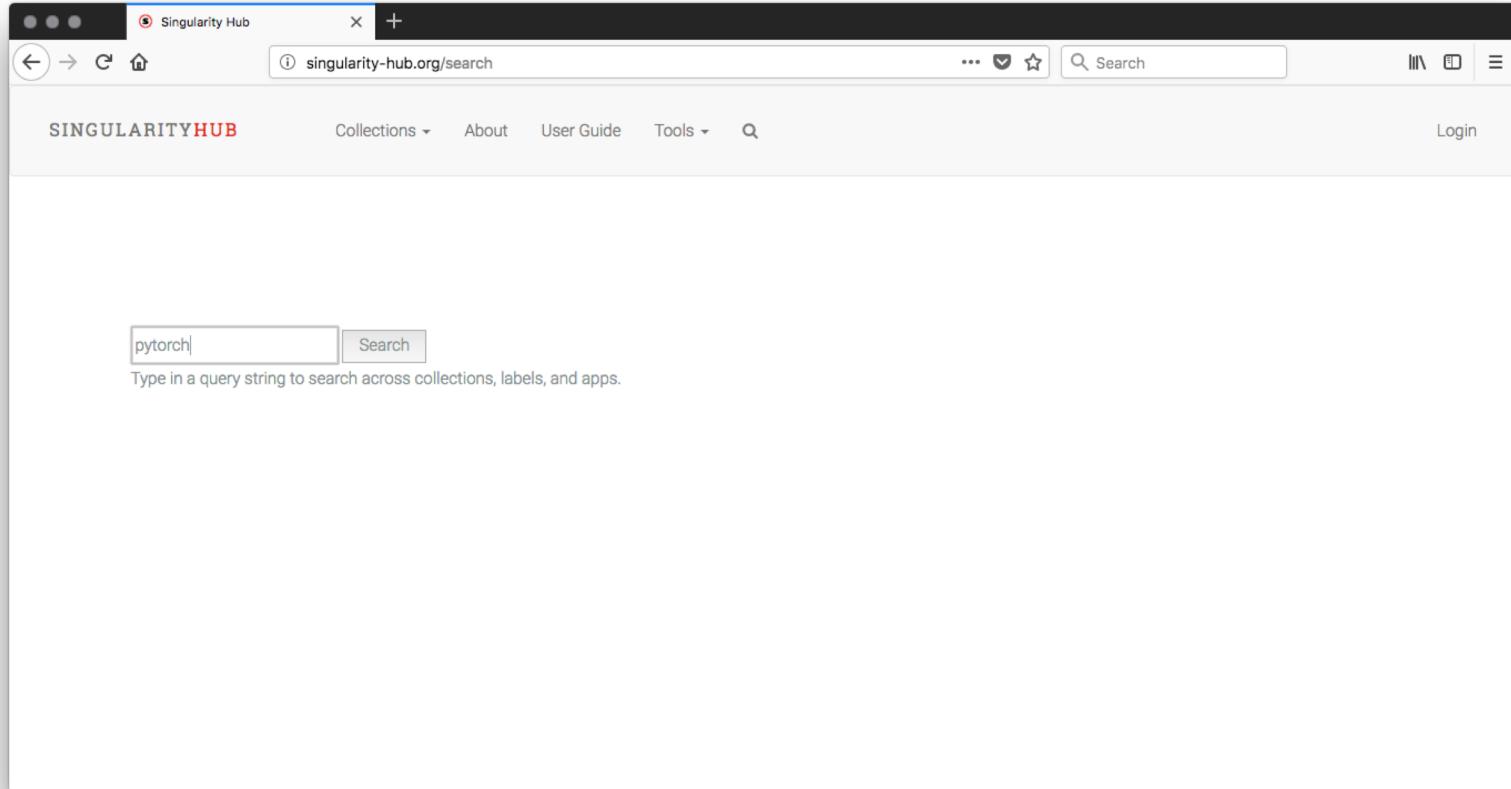
```
ubuntu@si2018:~/singularity-hello-world$ scp -p hello.simg \
etrain101@comet-ln2.sdsc.edu:/home/etrain101
hello.simg                                         100%    35MB   2.2MB/s   00:16
ubuntu@si2018:~/singularity-hello-world$
```

Using SingularityHub





<https://singularity-hub.org/>



<https://singularity-hub.org/search>

Tags

Labels

Found 8 collections

1. rses-singularity/tfgpu-theano-pytorch-keras	Containers: 1	Modified Date Feb. 8, 2018, 10:58 a.m.
2. bbbbrie/xenial-pytorch-container	Containers: 1	Modified Date April 8, 2018, 9:07 p.m.
3. bermanmaxim/pytorch-latest-singularity	Containers: 1	Modified Date April 30, 2018, 9:44 a.m.
4. belledon/pytorch_sing	Containers: 4	Modified Date June 1, 2018, 11:19 a.m.
5. marcc-hpc/pytorch	Containers: 2	Modified Date June 25, 2018, 4:09 p.m.
6. mcw-rcc/pytorch	Containers: 1	Modified Date July 12, 2018, 3:56 p.m.
7. Hao-Tju/pytorch-sing	Containers: 1	Modified Date July 20, 2018, 6:11 a.m.

The screenshot shows a web browser window with the URL <https://singularity-hub.org/collections/312>. The page title is "Singularity Hub". The main content area displays a collection named "marcc-hpc/pytorch". Below the name, it says "Singularity Container for PyTorch". There are two red buttons labeled "SINGULARITY" and "PYTORCH". To the right is a GitHub logo. Below the container name are two tabs: "SUPPLEMENTARY" (with a dropdown arrow) and "USAGE". Under "Builds", there are two rows of build information:

uri	Recipe	Status	Tag (Branch)	Date
marcc-hpc/pytorch:0.5.0	Singularity 0.5.0	COMPLETE	0.5.0 (0.5.0)	June 26, 2018, 7:46 a.m. build
marcc-hpc/pytorch:latest	Singularity	COMPLETE	latest (0.4.0)	May 30, 2018, 7:30 a.m. build

<https://singularity-hub.org/collections/312>

Integrating GitHub and SingularityHub



The screenshot shows a GitHub user profile for the account `hpcdevops`. The profile page includes a large cartoon portrait of a man with glasses and a beard. The main navigation bar at the top has links for Pull requests, Issues, Marketplace, and Explore. Below the navigation, there are tabs for Overview, Repositories (5), Stars (0), Followers (1), and Following (0). The Overview tab is selected. Under the Overview tab, there is a section for Pinned repositories, which lists four repositories: `singularity-hello-world`, `singularity-cloudmesh`, `comet-ompi`, and `tensorflow-gpu-nih`. Each pinned repository card includes a brief description and a language badge. Below the pinned repositories, there is a section for Organizations, showing one organization: SDSC. There is also a chart showing contributions over the last year.

<https://github.com/hpcdevops>

Simple hello world container for Singularity

18 commits 2 branches 1 release 2 contributors

Branch: master New pull request Create new file Upload files Find file Clone or download

tcooper Revert use of /code directory and HELLO_BASE Latest commit c69c285 4 days ago

LICENSE Initial commit a year ago

README.md Update README.md 5 days ago

Singularity Revert use of /code directory and HELLO_BASE 4 days ago

hello.sh Import environment during bootstrap test a year ago

README.md

singularity-hello-world hosted singularity-hub

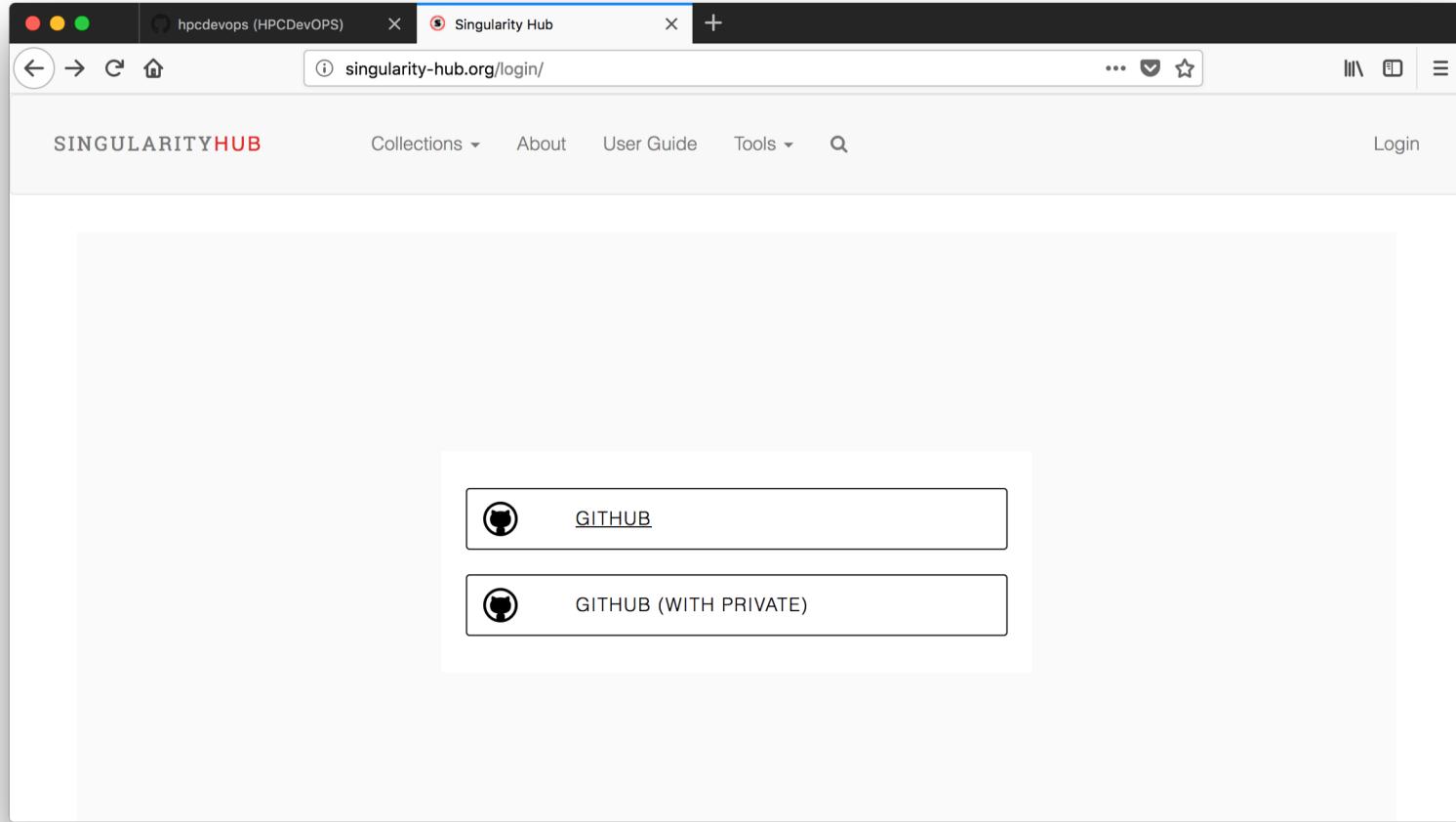
Very basic sample container definition for building on [Singularity Hub](https://singularity-hub.org/) (<https://singularity-hub.org/>) with re-build triggered on each push to the repository.

Pull the container directly with the following command...

```
% singularity pull shub://hpcdevops/singularity-hello-world:master
```

© 2018 GitHub, Inc. Terms Privacy Security Status Help Contact GitHub API Training Shop Blog About

<https://github.com/hpcdevops/singularity-hello-world>



<https://singularity-hub.org/login/>

hpcdevops (HPCDevOPS) X Authorize application X +

← → ⌂ ⌄ GitHub, Inc. (US) https://github.com/login/oauth/authorize?client_id=1d1dfb0d9f8f0 ... ⌂ ⌄ ⌄

The screenshot shows a GitHub OAuth authorization page. At the top, there are two circular icons: one with a red 'S' inside and another with a green checkmark. To the right of these is the GitHub logo. Below the icons, the text "Authorize Singularity Hub 2.0" is displayed. A large callout box contains the following information:

Singularity Hub 2.0 by vsoch
wants to access your hpcdevops account

Personal user data
Email addresses (read-only)

Repository webhooks and services
Admin access

Organization webhooks
Admin access

Commit statuses
Read and write access

Organizations and teams

The screenshot shows a web browser window for the Singularity Hub website (<https://www.singularity-hub.org/collections/my>). The header includes the Singularity Hub logo, navigation links for Collections, About, User Guide, Tools, and a search bar. A user profile for 'hpcdevops' is visible on the right. The main content area features a large icon of a cube with a small eye-like feature, followed by the text 'My Container Collections'. Below this is a red button labeled 'ADD A COLLECTION'. A note states that one collection is created for each connected Github repository, mentioning recipe file naming and build options. At the bottom, there's a search bar labeled 'Enter Keywords Here' and a table header with columns for Name, Builds, Description, Stars, Downloads, and Last Modified.

Name	Builds	Description	Stars	Downloads	Last Modified
------	--------	-------------	-------	-----------	---------------

<https://singularity-hub.org/collections/my>

A screenshot of a web browser window displaying the Singularity Hub website at <https://www.singularity-hub.org/collections/new>. The page title is "New Container Build". It features two container entries:

- hpcdevops/singularity-hello-world (represented by a blue icon)
- hpcdevops/tensorflow-gpu-nih (represented by a grey icon)

A red "SUBMIT QUERY" button is located in the top right corner of the main content area.

<https://singularity-hub.org/collections/new>

The screenshot shows a web browser window with the following details:

- Title Bar:** Shows the title "Singularity Hub" and the URL "https://www.singularity-hub.org/collections/1373".
- Header:** Includes the "SINGULARITYHUB" logo, navigation links for "Collections", "About", "User Guide", "Tools", and a search bar.
- Collection Details:** The collection is named "hpcdevops/singularity-hello-world".
 - Description: "Simple hello world container for Singularity"
 - Icons: A yellow star and a red GitHub icon.
- Buttons:** "SUPPLEMENTARY", "SETTINGS", and a refresh icon.
- Text:** A note explaining the automated build process, mentioning "commit", "refresh automatically", "deleted all of your containers", "commit again", "change your collection", "manual trigger", and "enable additional branches".
- Social Sharing:** Icons for GitHub, Facebook, and Twitter.

<https://singularity-hub.org/collections/1373>

The screenshot shows a web browser window with the URL <https://www.singularity-hub.org/collections/1373>. The page displays a container named "hpcdevops/singularity-hello-world". The container is described as a "Simple hello world container for Singularity". It has tabs for "SUPPLEMENTARY", "SETTINGS", "USAGE", and a copy icon. Below the tabs, there are sections for "Builds" and "COMMIT". The "Builds" section lists one build entry:

uri↓	Recipe	Status	Tag (Branch)	Date	
	hpcdevops/singularity-hello-w...	Singularity	RUNNING	latest (master)	July 27, 2018, 7:13 p.m. commit

At the bottom, there are links for "Rows per page: 50" and "1-1 of 1".

<https://singularity-hub.org/collections/1373>

The screenshot shows a web browser window with the URL <https://www.singularity-hub.org/collections/1373>. The page title is "Singularity Hub". The main content area displays a collection named "hpcdevops/singularity-hello-world". Below the name, a description reads "Simple hello world container for Singularity". There are two social sharing icons: a yellow star and a red GitHub icon. Below the description are four buttons: "SUPPLEMENTARY", "SETTINGS", "USAGE", and a refresh icon. Under the heading "Builds COMMIT", there is a table with one row. The columns are "uri", "Recipe", "Status", "Tag (Branch)", and "Date". The "uri" column shows a truncated URL "hpcdevops/singularity-hello-w...". The "Recipe" column shows "Singularity" with a cloud icon. The "Status" column is a green button labeled "COMPLETE". The "Tag (Branch)" column is "latest (master)". The "Date" column is "July 27, 2018, 7:13 p.m. commit". At the bottom of the table, there are links for "Rows per page: 50" and "1 - 1 of 1".

uri	Recipe	Status	Tag (Branch)	Date
hpcdevops/singularity-hello-w...	Singularity	COMPLETE	latest (master)	July 27, 2018, 7:13 p.m. commit

<https://singularity-hub.org/collections/1373>

The screenshot shows a web browser window with the following details:

- Title Bar:** Shows the title "Singularity Hub" and the URL "https://www.singularity-hub.org/collections/1373/usage".
- Header:** Features the "SINGULARITYHUB" logo, navigation links for "Collections", "About", "User Guide", "Tools", and a search bar.
- Collection Details:** Displays the repository name "hpcdevops/singularity-hello-world" in red text, with a "Usage" link and a GitHub icon.
- Usage Instructions:** A section titled "Pull" provides commands to pull the container:

```
singularity pull shub://hpcdevops/singularity-hello-world  
singularity pull --name customname.img shub://hpcdevops/singularity-hello-world  
singularity pull --commit shub://hpcdevops/singularity-hello-world  
singularity pull --hash shub://hpcdevops/singularity-hello-world
```
- Singularity Global Client Examples:** A section titled "Singularity Global Client Examples" provides commands for the Singularity global client:

```
registry pull hpcdevops/singularity-hello-world  
registry search hpcdevops/singularity-hello-world  
registry record hpcdevops/singularity-hello-world
```

<https://singularity-hub.org/collections/1373/usage>

hpcdevops (HPCDevOPS) X Singularity Hub X +

ADD A COLLECTION

One collection is created for each connected Github repository. In that collection, several containers will automatically be built: one for each uniquely named recipe file found in the master branch of the Github repository.

Read more about [recipe file naming](#) or [build options](#).

Enter Keywords Here

Name	Builds	Description	Stars	Downloads	Last Modified
hpcdevops/singularity-hello-world	1	Simple hello world container for Singularity	0	1	2018-07-27
hpcdevops/hello-world	1	testing container for pushing to singularity-hub	0	2	2018-07-27
hpcdevops/singularity-cloudmesh	1	Cloudmesh client container for Singularity	0	8	2018-07-27
hpcdevops/comet-ompi	1	Singularity container definition for OMPI demo on Comet	0	1	2018-07-27

Rows per page: 50

1 -4 of 4

<https://singularity-hub.org/collections/my>

Running Singularity on Comet

Singularity Basics

1. bash

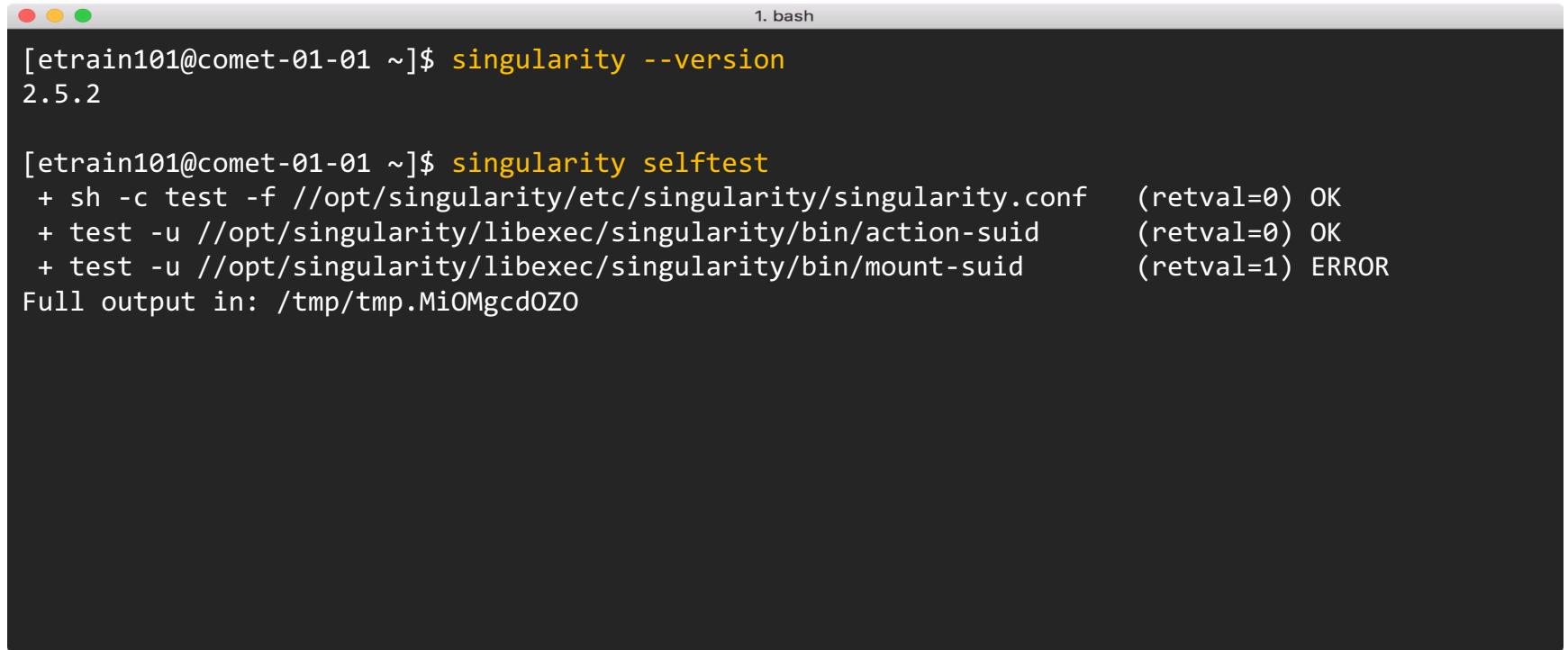
```
[etrain101@comet-01-01 ~]$ which singularity
/usr/bin/which: no singularity in
(/opt/gnu/gcc/bin:/opt/gnu/bin:/opt/mvapich2/intel(ib/bin:/opt/intel/composer_xe_2013_sp1.2.144/
bin/intel64:/opt/intel/composer_xe_2013_sp1.2.144/mpirt/bin/intel64:/opt/intel/composer_xe_2013_
sp1.2.144/debugger/gdb/intel64_mic/bin:/usr/lib64/qt-
3.3/bin:/usr/local/bin:/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/sbin:/opt/ibutils/bin:/usr/java/
latest/bin:/opt/pdsh/bin:/opt/rocks/bin:/opt/rocks/sbin:/opt/sdsc/bin:/opt/sdsc/sbin:/home/etrain101/bin)

[etrain101@comet-01-01 ~]$ module load singularity

[etrain101@comet-01-01 ~]$ which singularity
/opt/singularity/bin/singularity

[etrain101@comet-01-01 ~]$
```

Singularity Basics



A terminal window titled "1. bash" displaying command-line output. The output shows the Singularity version and the results of a self-test.

```
[etrain101@comet-01-01 ~]$ singularity --version
2.5.2

[etrain101@comet-01-01 ~]$ singularity selftest
+ sh -c test -f //opt/singularity/etc/singularity/singularity.conf      (retval=0) OK
+ test -u //opt/singularity/libexec/singularity/bin/action-suid          (retval=0) OK
+ test -u //opt/singularity/libexec/singularity/bin/mount-suid           (retval=1) ERROR
Full output in: /tmp/tmp.MiOMgcdOZO
```

Singularity Basics

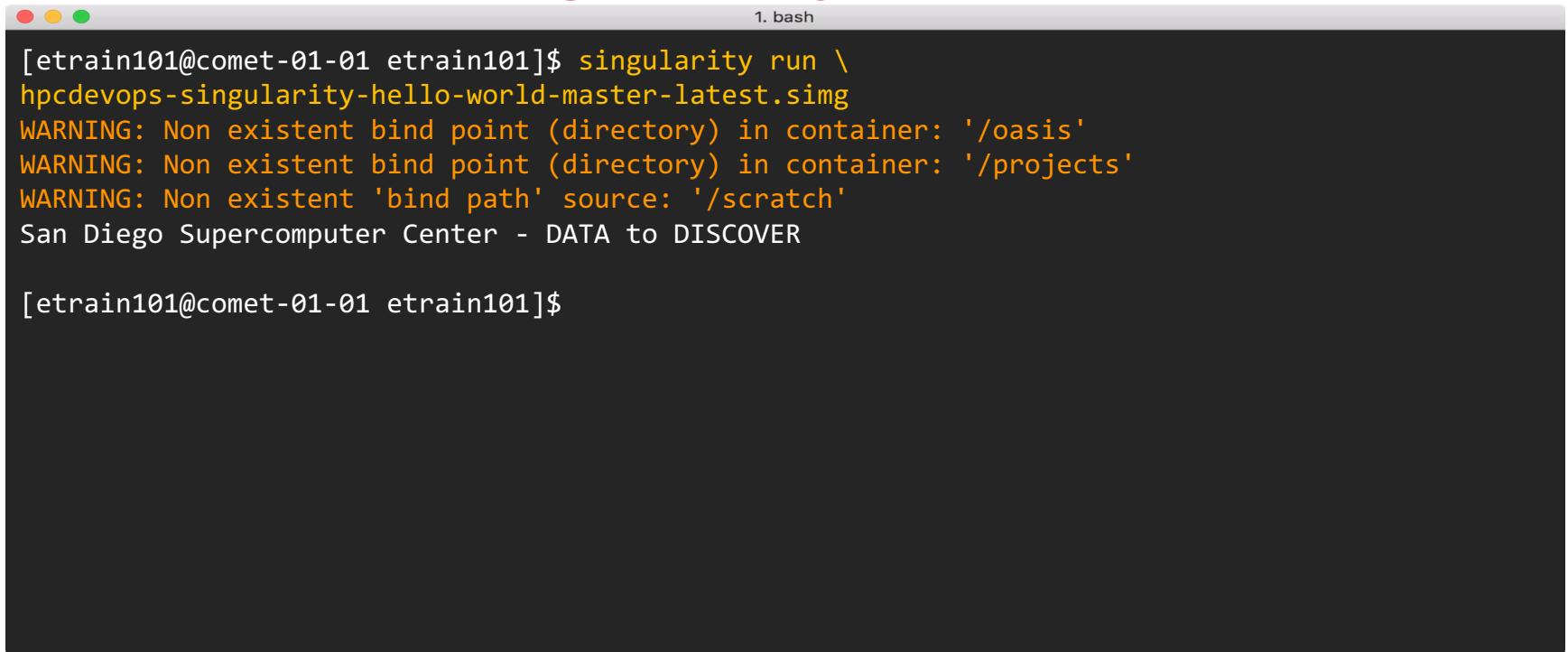
```
1. bash

[etrain101@comet-01-01 ~]$ mkdir -p /dev/shm/${USER}
[etrain101@comet-01-01 ~]$ chmod 750 /dev/shm/${USER}
[etrain101@comet-01-01 ~]$ cd /dev/shm/${USER}
[etrain101@comet-01-01 etrain101]$ df -hP .
Filesystem      Size  Used Avail Use% Mounted on
tmpfs          63G    0   63G   0% /dev/shm

[etrain101@comet-01-01 etrain101]$ singularity pull shub://hpcdevops/singularity-hello-world
Progress |=====| 100.0%
Done. Container is at: /dev/shm/etrain101/hpcdevops-singularity-hello-world-master-latest.simg

[etrain101@comet-01-01 etrain101]$
```

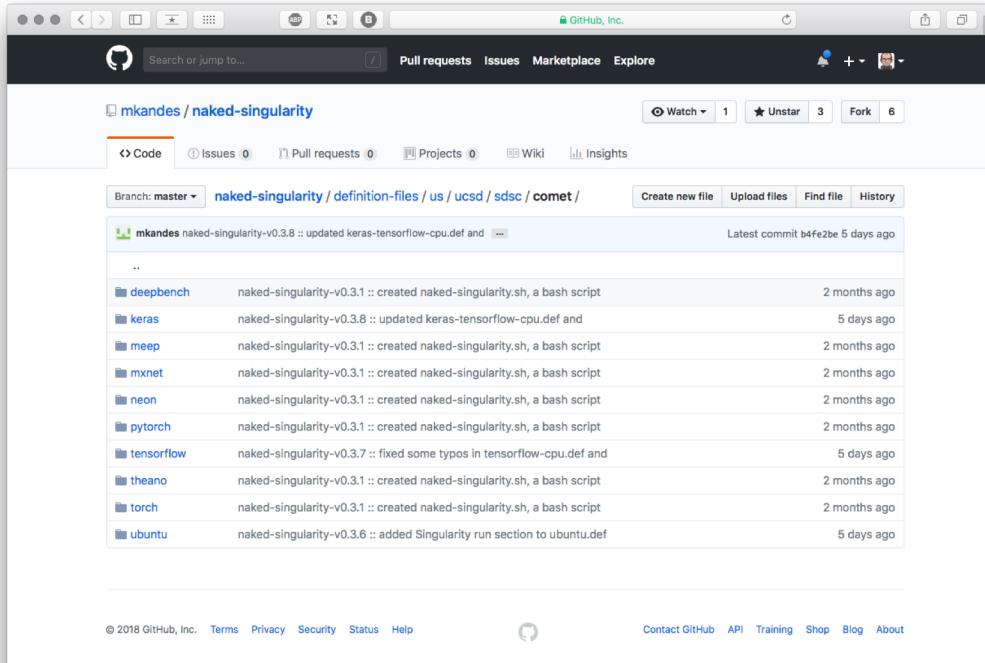
Singularity Basics

A screenshot of a terminal window titled "1. bash". The window shows a command being run to execute a Singularity container. The command is: [etrain101@comet-01-01 etrain101]\$ singularity run \ hpcdevops-singularity-hello-world-master-latest.simg. The output of the command includes several WARNING messages about non-existent bind points and a source path, followed by the text "San Diego Supercomputer Center - DATA to DISCOVER".

```
[etrain101@comet-01-01 etrain101]$ singularity run \
hpcdevops-singularity-hello-world-master-latest.simg
WARNING: Non existent bind point (directory) in container: '/oasis'
WARNING: Non existent bind point (directory) in container: '/projects'
WARNING: Non existent 'bind path' source: '/scratch'
San Diego Supercomputer Center - DATA to DISCOVER

[etrain101@comet-01-01 etrain101]$
```

Singularity Images



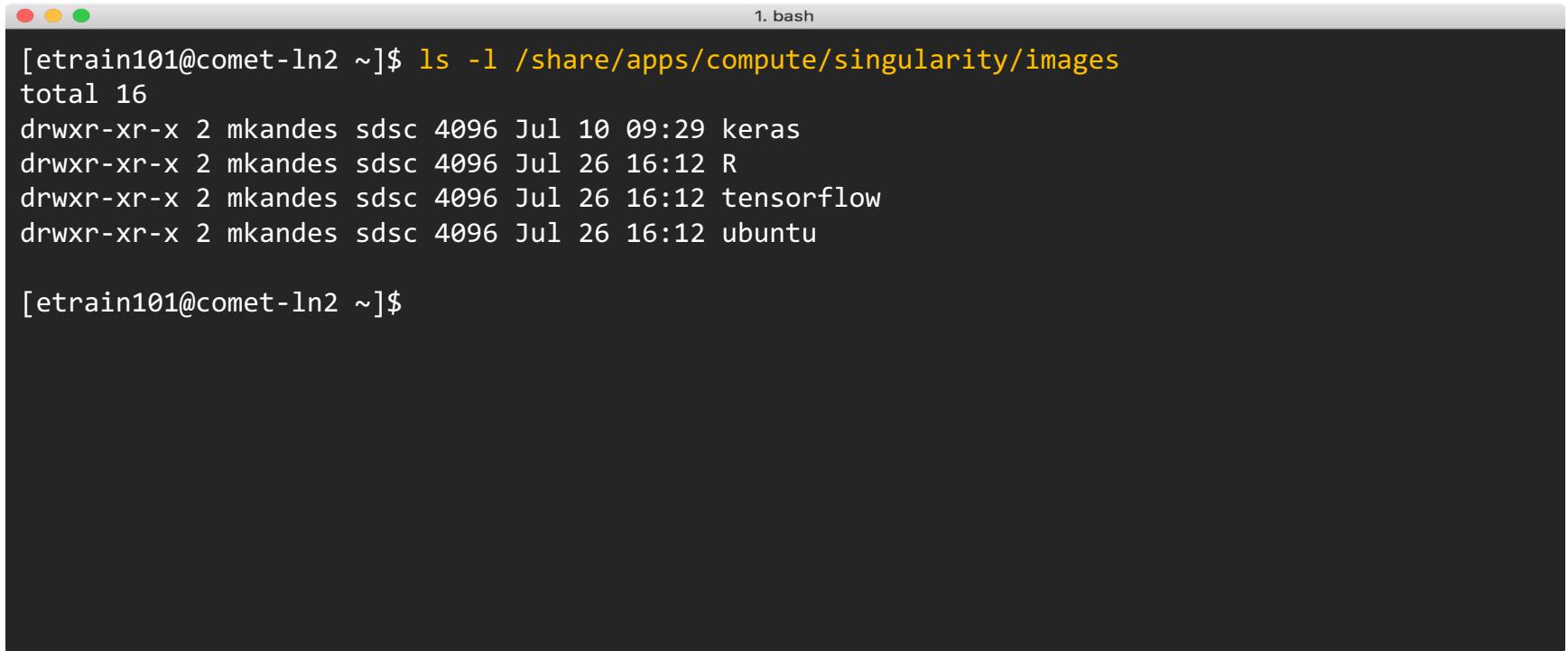
<https://github.com/mkandes/naked-singularity/>

Singularity Images

```
ubuntu@si2018:~/naked-singularity/definition-files/us/ucsd/sdsc/comet/tensorflow$ 1. bash
time sudo singularity build tensorflow-gpu.simg tensorflow-gpu.def
Using container recipe deffile: tensorflow-gpu.def
Sanitizing environment
Adding base Singularity environment to container
I: Retrieving InRelease
...snip...
After this operation, 39.9 MB of additional disk space will be used.
Get:1 http://us.archive.ubuntu.com/ubuntu xenial/main amd64 python-decorator all 4.0.6-1 [9326
B]
Get:2 http://us.archive.ubuntu.com/ubuntu xenial/main amd64 libwebp5 amd64 0.4.4-1 [165 kB]
3% [2 libwebp5 0 B/165 kB 0%]
^C

real 76m55.791s
user 4m35.428s
sys 2m35.072s
```

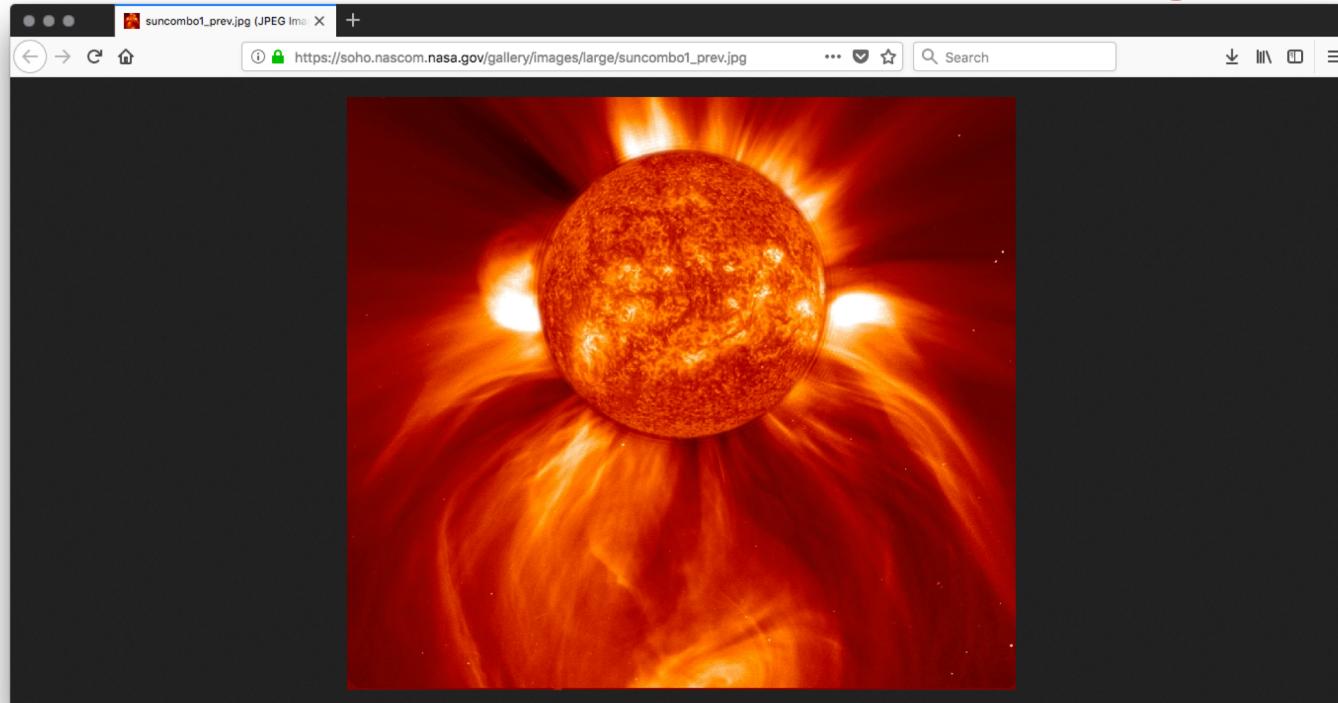
Singularity Images

A screenshot of a terminal window titled "1. bash". The window shows a file listing from a Linux command-line interface. The output of the "ls -l /share/apps/compute/singularity/images" command is displayed, showing four files: keras, R, tensorflow, and ubuntu, all owned by mkandes and sdsc, with modification dates between July 10 and 26.

```
[etrain101@comet-ln2 ~]$ ls -l /share/apps/compute/singularity/images
total 16
drwxr-xr-x 2 mkandes sdsc 4096 Jul 10 09:29 keras
drwxr-xr-x 2 mkandes sdsc 4096 Jul 26 16:12 R
drwxr-xr-x 2 mkandes sdsc 4096 Jul 26 16:12 tensorflow
drwxr-xr-x 2 mkandes sdsc 4096 Jul 26 16:12 ubuntu

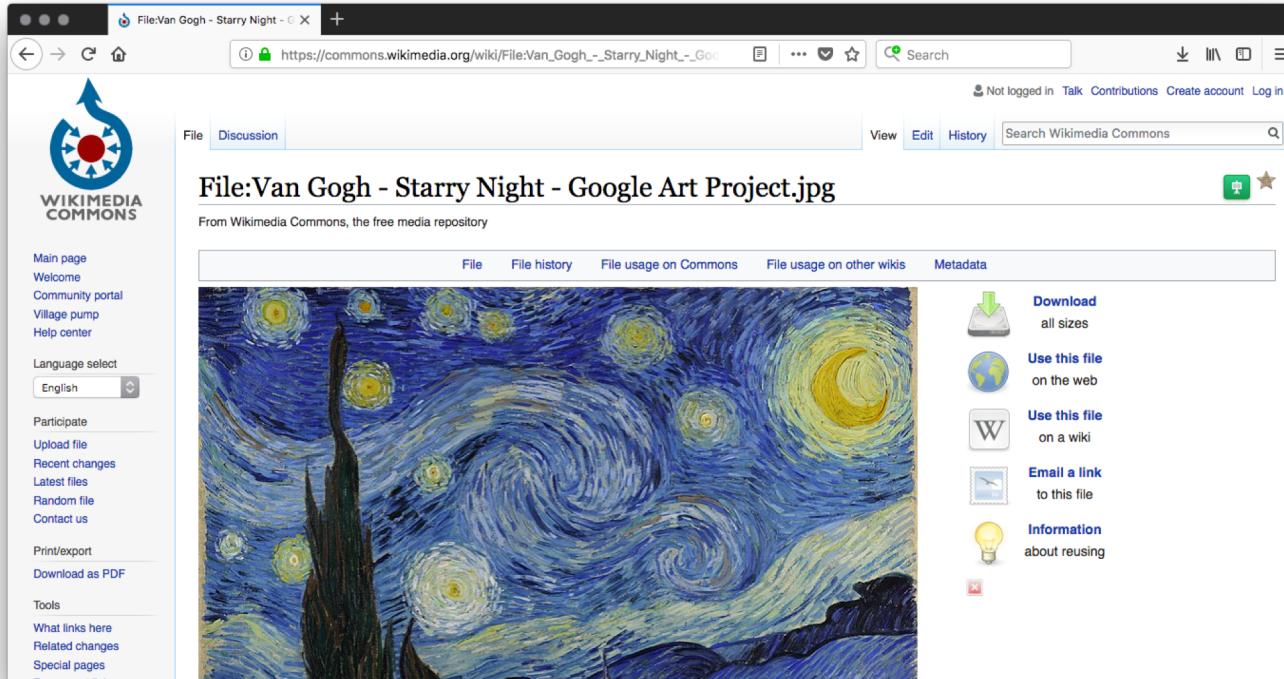
[etrain101@comet-ln2 ~]$
```

Take a NASA SOHO image...



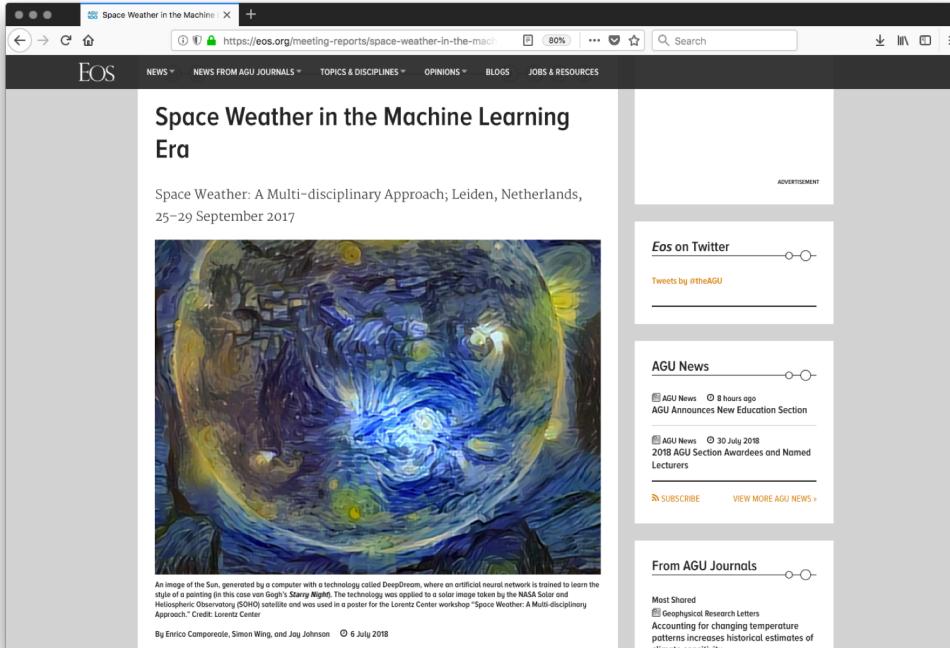
https://soho.nascom.nasa.gov/gallery/images/large/suncombo1_prev.jpg

...and ‘stylize’ it with...



https://commons.wikimedia.org/wiki/File:VanGogh-starry_night.jpg

...NOT an original idea...



<https://eos.org/meeting-reports/space-weather-in-the-machine-learning-era>

Train the model...

```
1. bash  
[etrain101@comet-ln2 pytorch-gpu]$ grep srun ${PWD}/fast_neural_style_train.run -B2 -A8  
echo -e "\n---CUT HERE---\n"  
  
srun singularity exec --nv ${SINGULARITY_IMAGE_DIR}/pytorch-gpu.simg \  
python /opt/pytorch-examples/fast_neural_style/neural_style/neural_style.py \  
train \  
--dataset "${LOCAL_SCRATCH}" \  
--style-image ${file_dir}/${file_name}.${file_ext} \  
--save-model-dir ${model_dir} \  
--epochs 5 \  
--cuda 1  
  
ret=$?  
  
echo -e "\n---CUT HERE---\n"  
  
[etrain101@comet-ln2 pytorch-gpu]$
```

Submit the training job... and wait...

```
1. bash  
[etrain101@comet-ln2 pytorch-gpu]$ sbatch --reservation=SI2018DAY1 \  
 ${PWD}/fast_neural_style_train.run \  
 ${PWD}/van_gogh_starry_night.jpg \  
 ${PWD}/pytorch-examples/fast_neural_style/saved_models  
Submitted batch job 18258600  
  
[etrain101@comet-ln2 pytorch-gpu]$ squeue  
JOBID PARTITION      NAME      USER ST      TIME  NODES NODELIST(REASON)  
 18258600      gpu  fast_neu etrain10 R      0:15      1 comet-30-18  
  
[etrain101@comet-ln2 pytorch-gpu]$ sacct -X -P -o Partition,JobName,NNodes,NCPUS,ReqGRES,Elapsed  
-j 18258600 | column -s\| -t  
Partition      JobName          NNodes   NCPUS   ReqGRES   Elapsed  
gpu-shared    fast_neural_style_train  1        6     gpu:1    22:29:25  
  
[etrain101@comet-ln2 pytorch-gpu]$
```



Stylize the content... quick...

```
1. bash  
[etrain101@comet-ln2 pytorch-gpu]$ grep srun ${PWD}/fast_neural_style_stylize.run -B2 -A11  
echo -e "\n---CUT HERE---\n"  
  
srun singularity exec ${SINGULARITY_IMAGE_DIR}/pytorch-gpu.simg \  
python /opt/pytorch-examples/fast_neural_style/neural_style/neural_style.py \  
eval \  
--content-image ${file_dir}/${file_name}.${file_ext} \  
--model ${model_dir}/${model_name}.${model_ext} \  
--output-image ${file_dir}/${file_name}_${model_name}.${file_ext} \  
--content-scale 2 \  
--cuda 0  
  
ret=$?  
  
echo -e "\n---CUT HERE---\n"  
  
[etrain101@comet-ln2 pytorch-gpu]$
```

Submit the styling job...

```
1. bash  
[etrain101@comet-ln2 pytorch-gpu]$ sbatch --reservation=SI2018DAY1 \  
 ${PWD}/fast_neural_style_stylize.run \  
 ${PWD}/soho_suncombo1_prev.jpg \  
 ${PWD}/pytorch-examples/fast_neural_style/saved_models/van_gogh_starry_night.pth  
Submitted batch job 18258608  
  
[etrain101@comet-ln2 pytorch-gpu]$ squeue  
      JOBID PARTITION      NAME      USER ST      TIME  NODES NODELIST(REASON)  
 18258608    compute  fast_neu  etrain10  R      0:03      1 comet-10-43  
  
[etrain101@comet-ln2 pytorch-gpu]$ $ sacct -X -P \  
 -o Partition,JobName,NNodes,NCPUS,ReqGres,Elapsed -j 18258608 | column -s\| -t  
Partition  JobName          NNodes  NCPUS  ReqGRES  Elapsed  
compute    fast_neural_style_stylize  1        24      00:00:04  
  
[etrain101@comet-ln2 pytorch-gpu]$
```



Observe the result...



A terminal window titled "1. bash" displays the following commands and output:

```
[etrain101@comet-ln2 pytorch-gpu]$ ls -ltr *.jpg
-rw-r--r-- 1 etrain101 gue998 309334 Aug  2 15:15 soho_suncombo1_prev.jpg
-rw-r--r-- 1 etrain101 gue998 355826 Aug  2 15:15 van_gogh_starry_night.jpg
-rw-r--r-- 1 etrain101 gue998 34843 Aug  2 15:20 soho_suncombo1_prev_van_gogh_starry_night.jpg

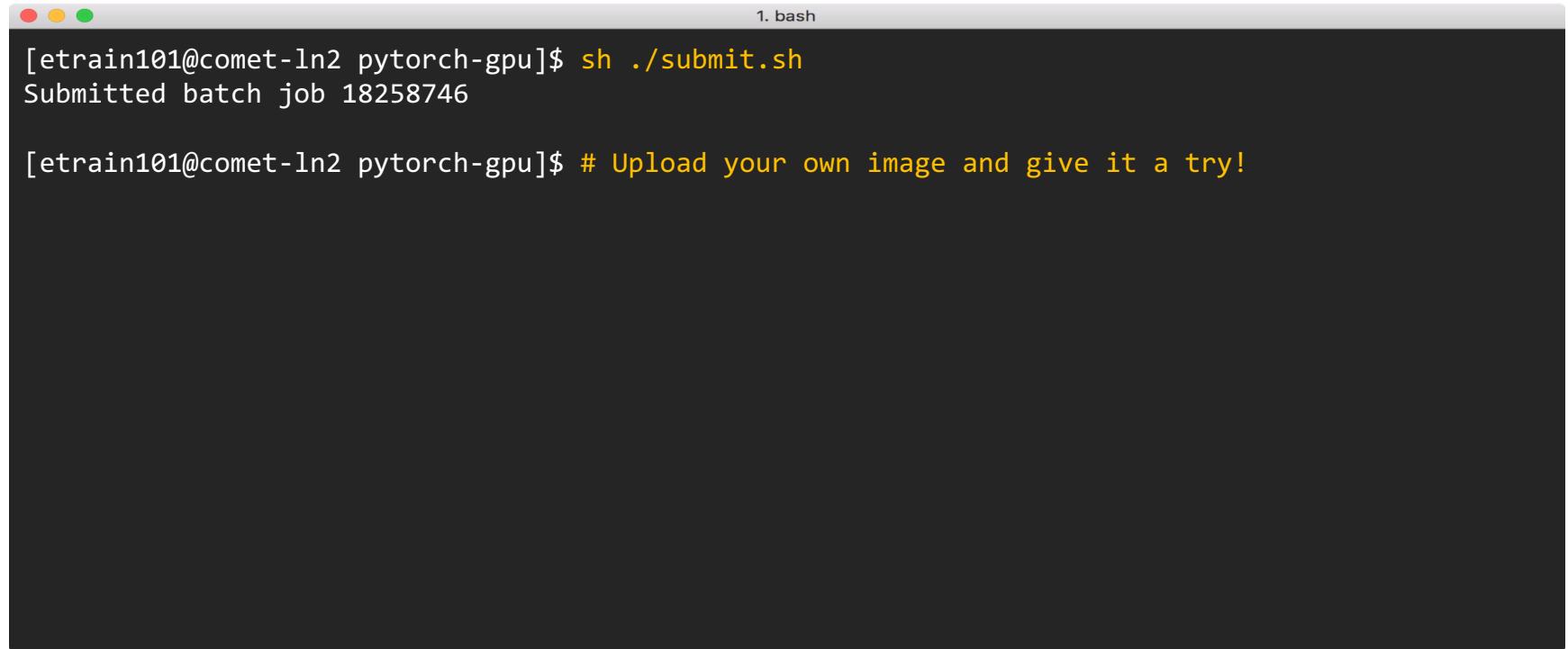
[etrain101@comet-ln2 pytorch-gpu]$ display soho_suncombo1_prev_van_gogh_starry_night.jpg

[etrain101@comet-api pytorch-gpu]$
```

Let's do it...

```
1. bash  
[etrain101@comet-ln2 ~]$ cp -r /share/apps/examples/SI2018/Singularity/jobs ./  
  
[etrain101@ comet-ln2 ~]$ cd jobs/pytorch-gpu/  
  
[etrain101@comet-ln2 pytorch-gpu]$ ls  
fast_neural_style_stylize.18258619.comet-19-58.out  fast_neural_style_train.run  
soho_suncombo1_prev.jpg                            van_gogh_starry_night.jpg  
fast_neural_style_stylize.run                      pytorch-examples                submit.sh  
  
[etrain101@comet-api pytorch-gpu]$ cat ./submit.sh  
#!/bin/bash  
  
sbatch --reservation=SI2018DAY1 ${PWD}/fast_neural_style_stylize.run  
${PWD}/soho_suncombo1_prev.jpg ${PWD}/pytorch-  
examples/fast_neural_style/saved_models/van_gogh_starry_night.pth  
  
[etrain101@comet-ln2 pytorch-gpu]$
```

Let's do it...



A screenshot of a terminal window titled "1. bash". The window shows a command-line session where a user named "etrain101" is running a script to submit a job to a "pytorch-gpu" cluster. The output indicates that the job has been submitted with the ID 18258746. A note at the bottom encourages users to upload their own images.

```
[etrain101@comet-ln2 pytorch-gpu]$ sh ./submit.sh
Submitted batch job 18258746

[etrain101@comet-ln2 pytorch-gpu]$ # Upload your own image and give it a try!
```



More on DeepDream

- Try your hand building a Caffe Singularity container and use it along with the iPython Notebook found here...

<https://github.com/google/deepdream/blob/master/dream.ipynb>

- Or Google DeepDream and use an online generator...

Thanks!

- Special thanks to **Martin Kandes** for production of the pytorch-gpu Singularity image and help with the `fast_neural_style` PyTorch workflow example.

https://www.sdsc.edu/support/user_guides/tutorials/running_singularity_on_comet.html