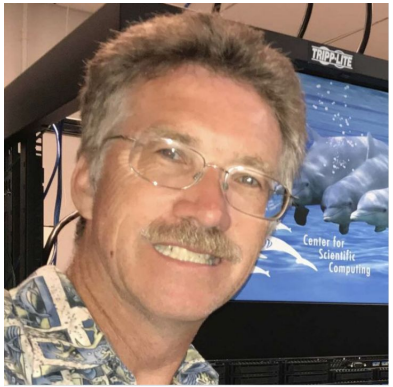
Apptainer / Singularity Containers On the Clusters

W00t! UC Santa Barbara!

Ye Olde People Introductions



Paul Weakliem, PhD
Co-Director
Center for Scientific Computing &
California Nanosystems Institute
Eling 3231
weakliem@cnsi.ucsb.edu

Fuzzy Rogers
That guy in the MRL
Center for Scientific Computing &
Materials Research Laboratory
MRL 2066B
fuz@ucsb.edu

Yu-Chieh “Jay” Chi, PhD
Research Computing Consultant
Center for Scientific Computing &
Enterprise Technology Services
Elings 3229
jaychi@ucsb.edu

CSC Center for Scientific Computing

CNSI

UC SANTA BARBARA MRL Materials Research Laboratory
NSF Materials Research Science and Engineering Center [DMR 1720256]

ENTERPRISE TECHNOLOGY SERVICES

Ack!

- Acknowledgements - https://csc.cnsi.ucsb.edu/publications

Please acknowledge the CSC in publications and presentations if you are using our facility's computational resources (including staff involvement) in your research.

"We acknowledge support from the Center for Scientific Computing from the CNSI, MRL: an NSF MRSEC (DMR-1720256) and NSF CNS- 1725797."

Caveat Emptor

Here is where I absolve myself from all blame by stating that the soon to be aforementioned was to the best of my knowledge.

What is this thing you call a container?

• Containers are linux software environments where the user can have control over everything but the kernel.

• Apptainer / Singularity containers can be used to package entire scientific workflows, software and libraries, and even data, in an immutable format. This means that you don’t have to ask your cluster admin to install anything for you - you can create a software workflow in a Apptainer / Singularity container and run it on the clusters.

• With Docker integration, one can utilize proven shared containers as if they were applications (that can contain multiple applications).

Apptainer / Singularity on Pod

- https://apptainer.org/docs/user/latest/ ←- docs and info
- module load apptainer
  (or singularity/3.5.2 or singularity/2.6)
- Binaries of apptainer and singularity (and their builds) are in /sw/singularity
- Images are created by ‘Definition’ (.def) files and are very bare bones - you need to ask for the packages you want installed
- The resulting image files (.sif) are immutable

The one command to execute.

Such an immutable kitty!

Apptainer & Docker

- Apptainer can pull and transmogrify docker containers to create a .sif (singularity image format) file/image

  apptainer pull docker://ghcr.io/apptainer/lolcow

  …exciting things happen …


```
INFO:    Converting OCI blobs to SIF format
INFO:    Starting build...
Getting image source signatures
Copying blob 5ca731fc36c2 done
Copying blob 16ec32c2132b done
Copying config fd0daa4d89 done
Writing manifest to image destination
Storing signatures
2023/02/08 14:37:49  info unpack layer:
sha256:16ec32c2132b43494832a05f2b02f7a822479f8250c173d0ab27b3de78b2f058
2023/02/08 14:37:50  info unpack layer:
sha256:5ca731fc36c28789c5ddc3216563e8bfca2ab3ea10347e07554ebba1c953242e
INFO:    Creating SIF file…
```

Apptainer & Docker

- Look at the SIF
  -bash-4.2$ ls -lh
  …
  -rwxr-xr-x 1 fuz seshadri 72M Feb 8 14:37 lolcow_latest.sif
- Run the container with input from the outside and then exit back to CentOS 7 Pod:
  -bash-4.2$ apptainer exec lolcow_latest.sif cowsay moo

Program to run in container

Input for that program

```
 _____
< moo >
 -----
        \   ^__^
         \  (oo)\_______
            (__)\       )\/\
                ||----w |
                ||     ||
```

←– the output

<- Clarus the Dogcow
1983, Apple (not created by the container)

Apptainer & Docker

- -bash-4.2$ apptainer exec lolcow_latest.sif cowsay moo
  -bash-4.2$ apptainer run lolcow_latest.sif cowsay moo

```
-bash-4.2$ apptainer run lolcow_latest.sif cowsay
 _____________________________
< Sat Feb 11 13:22:51 PST 2023 >
 -----------------------------
        \  ^__^
         \ (oo)\_______
           (__)\       )\/\
              ||----w |
              ||     ||
-bash-4.2$ apptainer exec lolcow_latest.sif cowsay moo
 _____
< moo >
 -----
        \  ^__^
         \ (oo)\_______
           (__)\       )\/\
              ||----w |
              ||     ||
```

Runs the commands under %runscript in the .def (Definition) file - a bit of a black box if you cannot see how the container was defined.

This command will launch an Apptainer container and execute a runscript if one is defined for that container. The runscript is a metadata file within the container that contains shell commands. If the file is present (and executable) then this command will execute that file within the container automatically. All arguments following the container name will be passed directly to the runscript.

That's a cat.
That's a cow.

exec just executes the program in the container with the input from the end

Apptainer & Docker

Let’s look a bit at our .sif image - we can shell into it:

-bash-4.2$ **apptainer shell lolcow_latest.sif**

Apptainer>

Apptainer> cat /etc/debian_version

bullseye/sid

Apptainer> df -h

Apptainer> which cowsay

/usr/games/cowsay

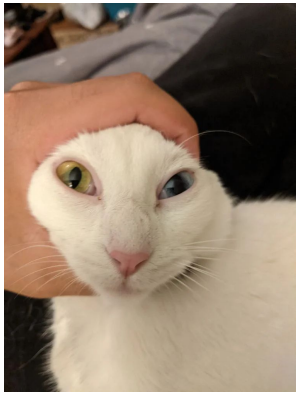
Apptainer> set | grep games ←—-- ‘set’ shows your environment variables

PATH=/usr/games:/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/bin

Apptainer> exit

```
Filesystem      Size  Used Avail Use% Mounted on
overlay          16M   12K   16M   1% /
devtmpfs         94G     0   94G   0% /dev
tmpfs            94G   19M   94G   1% /dev/shm
/dev/md126      437G  128G  309G  30% /tmp
beegfs_nodev    655T  569T   87T  87% /home/fuz
tmpfs            16M   12K   16M   1% /etc/group
```

Apptainer & Docker



- Can mount other filesystems with the –bind flags:
  apptainer shell --bind /scratch,/sw lolcow_latest.sif
  Apptainer> df -h

```
Filesystem          Size  Used Avail Use% Mounted on
overlay              16M   12K   16M   1% /
devtmpfs             94G     0   94G   0% /dev
tmpfs                94G   19M   94G   1% /dev/shm
/dev/md126          437G  128G  309G  30% /tmp
beegfs_nodev        655T  569T   87T  87% /home/fuz
tmpfs                16M   12K   16M   1% /etc/group
10.0.50.249:/scratch 19T  8.4T  9.9T  46% /scratch
10.0.50.254:/sw     3.5T  1.8T  1.6T  53% /sw
/dev/loop0           72M   72M     0 100% /sw/singularity/apptainer/var/apptainer/mnt/session/rootfs
```

- Not everything you find in Docker easily turns into a .sif - just because you find a docker website with what you want does not mean it will be ‘easy’ to make an apptainer out of it. If you have docker installed, then you can try your hand at making an image and porting it over.
  For instance: https://hub.docker.com/r/nvaitc/ai-lab

← Obsequious cat

Building an Apptainer

- You can build your very own .sif container using .def files with all the packages you want that exist in base repositories (maybe non-base too, haven't looked much)

```
-bash-4.2$ more fuzcontainer.def
BootStrap: docker
From: ubuntu:20.04
%post
    apt-get -y update
    apt-get -y install cowsay vim bc python3
%environment
    export LC_ALL=C
    export PATH=/usr/games:$PATH
%runscript
    date | cowsay
%labels
    Author Fuz
```

I've chosen to install vim. Is an editor necessary? Probably not. But, you'll be surprised what isn't installed by default.

Pipe 'date' into cowsay - when run'd, this is what it runs

Build the .def with:

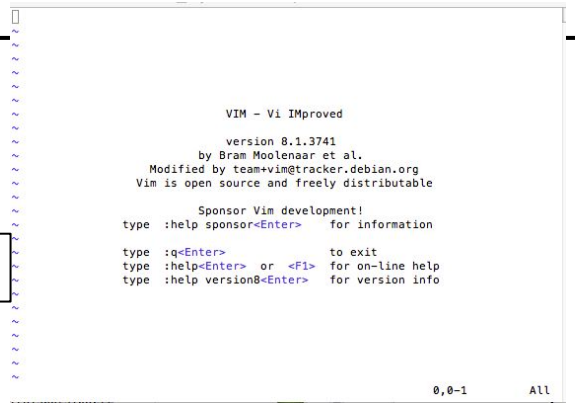
apptainer build fuzcontainer.sif fuzcontainer.def

Let's try vim in lolcow_latest.sif

```
bash-4.2$ apptainer shell --bind /scratch,/sw lolcow_latest.sif
Apptainer> vim
bash: vim: command not found
```

Now with fuzcontainer.sif

```
-bash-4.2$ apptainer shell --bind /scratch,/sw fuzcontainer.sif
Apptainer> vim
```



Building an Apptainer

Let’s play with the %runscript … what if I go… (modifying my .def file)

```
%runscript
    date | cowsay
    df -h | cowsay
    bc < bcinput
```

```
-bash-4.2$ cat bcinput
7 * 3.000482469859387459872934923
```

Build it … apptainer build fuzcontainer-bc.sif fuzcontainer.def

```
-bash-4.2$ apptainer run fuzcontainer-bc.sif
 _____________________________
< Mon Feb 13 10:11:36 PST 2023 >
 -----------------------------
        \   ^__^
         \  (oo)\_______
            (__)\       )\/\
                ||----w |
                ||     ||
 _____________________________
/ Filesystem Size Used Avail Use% Mounted \
| on overlay 16M 12K 16M 1% / devtmpfs    |
| 94G 0 94G 0% /dev tmpfs 94G 19M 94G 1%  |
| /dev/shm /dev/md126 437G 139G 298G 32%  |
| /tmp beegfs_nodev 655T 571T 85T 88%     |
| /home/fuz tmpfs 16M 12K 16M 1%          |
\ /etc/group                              /
 ------------------------------------------
        \   ^__^
         \  (oo)\_______
            (__)\       )\/\
                ||----w |
                ||     ||
21.003377289015712219110544461
```

Building an Apptainer

- You can build from Dockerfiles - but you gotta translate into apptainer syntax

  https://apptainer.org/docs/user/1.0/docker_and_oci.html#apptainer-definition-file-vs-dockerfile

  Here's the Dockerfile for BioPython

```
FROM ubuntu:16.04
MAINTAINER Tiago Antao <tra@popgen.net>

ENV DEBIAN_FRONTEND noninteractive
#We need this for phylip
RUN echo 'deb http://archive.ubuntu.com/ubuntu xenial multiverse' >> /etc/apt/sources.list \
                        && apt-get update \
                        && apt-get upgrade -y --force-yes \
                        && apt-get install -y --force-yes \
    build-essential \
    git \
    python3-numpy \
     wget \
     gcc \
     g++ \
     python3-dev \
     unzip \
     make \
     python3-matplotlib \
     python3-reportlab \
     python3-pip r-base \
     clustalw \
     fasttree \
     t-coffee python3-pil \
     bwa \
     ncbi-blast+ \
     emboss \
     clustalo \
     phylip \
     mafft \
        muscle \
        samtools \
        phyml \
        wise \
        raxml \
        language-pack-en \
        paml \
        probcons \
        python3-pandas \
        python3.5-dev \
        libxft-dev \
        && apt-get clean

#for Phylo_CDAO
# RUN pip3 install pip --upgrade
RUN pip3 install rdflib --upgrade \
    && pip3 install cython --upgrade \
    && pip3 install numpy --upgrade \
    && pip3 install Pillow --upgrade \
    && pip3 install matplotlib --upgrade \
    && pip3 install pandas --upgrade

#Manual software
RUN echo "export DIALIGN2_DIR=/tmp" >> .bashrc
```

… and it goes on and on and on

Turning this, by hand, into a modified BioPython .def would be a long process

Nicer to …. apptainer pull docker://biopython/biopython

But then you don't have any customization

Apptainer & GPUs

- Apptainer plays nicely with Pod's GPUs - use the development node pod-gpu for testing
- –nv (2 hyphens)
- Remember to send SLURM job file to gpu: sbatch -p gpu mygpustuff.job
- Apptainer is better than Singularity for interaction with GPUs

nv - the UCSB Jayich diamond research - https://www.10-9lab.com/spin-coherence/ (actually it stands for nvidia, not nitrogen vacancy)

Sidebar: So why ever use Singularity? My suggestion is to not use it.
Singularity can give you a writable container, in a relatively easy fashion, that you can manipulate to your liking. Apptainer can do that to - with the Sandbox function, but once you learn how to do something, it's sometimes easier to stick with it. Apptainer creates an entire subdirectory root filesystem of the container, whereas Singularity keeps it all inside its container.

```
-bash-4.2$ apptainer build --sandbox ubuntu/ docker://ubuntu
-bash-4.2$ cd ubuntu
-bash-4.2$ ls
bin  boot  dev  environment  etc  home  lib  lib32  lib64  libx32  media  mnt  opt  proc  root  run  sbin  singularity  srv  sys  tmp  usr  var
```

Apptainer & GPUs

As long as we're sidebarring:
If you already have a container saved locally, you can use it as a target to build a new container. This allows you to convert containers from one format to another. For example if you had a sandbox container called ubuntu/ and you wanted to convert it to a SIF container called myubuntu.sif you could:

$ apptainer build myubuntu.sif ubuntu/

Use care when converting a sandbox directory to the default SIF format. If changes were made to the writable container before conversion, there is no record of those changes in the Apptainer definition file rendering your container non-reproducible. It is a best practice to build your immutable production containers directly from an Apptainer definition file instead.

(shamelessly stolen from: https://apptainer.org/docs/user/main/build_a_container.html)

Apptainer & GPUs

Or: Let's pull a GPU thingy!

```
apptainer pull docker://tensorflow/tensorflow:latest-gpu
apptainer run --nv tensorflow_latest-gpu.sif
Apptainer> python
Python 3.6.8 |Anaconda, Inc.| (default, Dec 30 2018, 01:22:34)
[GCC 7.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>from tensorflow.python.client import device_lib
Traceback (most recent call last):
File "<stdin>", line 1, in <module>
ModuleNotFoundError: No module named 'tensorflow'
```

Ohh? What's this? Aha - it found the wrong python - it found my anaconda python....

```
Apptainer> which python
/home/fuz/anaconda3/bin/python
```

So - let's use the container's python that has TF

```
Apptainer> /bin/python3
Python 3.8.10 (default, Jun 22 2022, 20:18:18)
[GCC 9.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
                    from tensorflow.python.client import device_lib
….stuff…….
                    print(device_lib.list_local_devices())
…..stuff…..
```

Important! Your .bashrc may affect what the container sees. When you submit a job, you'd need /bin/python3 mypython.py

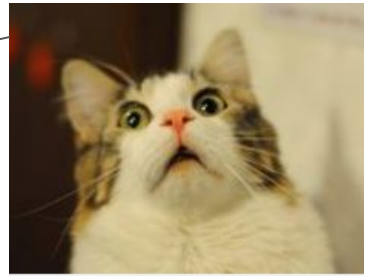
Let's see what the container sees for the GPUs

Apptainer & GPUs

Continuing the output, seeing the GPUs…..

```
-> device: 0, name: Tesla V100-PCIE-32GB, pci bus id: 0000:17:00.0, compute capability: 7.0
2023-02-09 12:24:25.069041: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1613] Created device /device:GPU:1 with 13779 MB memory:  -> device: 1, name: Tesla T4, pci bus
id: 0000:65:00.0, compute capability: 7.5
[name: "/device:CPU:0"
device_type: "CPU"
memory_limit: 268435456
locality {
}
incarnation: 8336112430592221785
xla_global_id: -1
, name: "/device:GPU:0"
device_type: "GPU"
memory_limit: 32473874432
locality {
bus_id: 1
links {
}
}
incarnation: 8868894900487111325
physical_device_desc: "device: 0, name: Tesla V100-PCIE-32GB, pci bus id: 0000:17:00.0, compute capability: 7.0"
xla_global_id: 416903419
, name: "/device:GPU:1"
device_type: "GPU"
memory_limit: 14449115136
locality {
bus_id: 1
links {
}
}
incarnation: 14753446127920954602
physical_device_desc: "device: 1, name: Tesla T4, pci bus id: 0000:65:00.0, compute capability: 7.5"
xla_global_id: 2144165316
]
```

This is pod-gpu login node, FYI



I know! I was surprised too.

Apptainer & GPUs

- Okay- this is all well and good, but let's do something SLURMy

  In my frantic preparation for this talk I decided to grab the TF "1st grader" example - it's all Paul's fault

My SLURM job script:

```
#!/bin/bash
# ask for 1 core on one node and 1 GPU
#SBATCH -N 1 --ntasks-per-node=1
#SBATCH --time=01:00:00
#SBATCH --partition=gpu
#SBATCH --gres=gpu:1

cd $SLURM_SUBMIT_DIR
module load apptainer
hostname
apptainer exec --nv tensorflow_latest-gpu.sif /bin/python3 teras-example.py
```

Umm, yeah- this is your friend If you use GPUs, you'll need that flag

Agitated cat sees the problem. Fuzzy did not.

My python file (teras-example.py) to run:

```
from tensorflow.python.client import device_lib
print(device_lib.list_local_devices())
import tensorflow as tf
print("TensorFlow version:", tf.__version__)
mnist = tf.keras.datasets.mnist

(x_train, y_train), (x_test, y_test) = mnist.load_data()
x_train, x_test = x_train / 255.0, x_test / 255.0
model = tf.keras.models.Sequential([
  tf.keras.layers.Flatten(input_shape=(28, 28)),
  tf.keras.layers.Dense(128, activation='relu'),
  tf.keras.layers.Dropout(0.2),
  tf.keras.layers.Dense(10)
])
predictions = model(x_train[:1]).numpy()
predictions) + '\n')
f.nn.softmax(predictions).numpy())
loss_fn = tf.keras.losses.SparseCategoricalCrossentropy(from_logits=True)
loss_fn(y_train[:1], predictions).numpy()
model.compile(optimizer='adam',
              loss=loss_fn,
              metrics=['accuracy'])
model.evaluate(x_test,  y_test, verbose=2)
probability_model = tf.keras.Sequential([
  model,
  tf.keras.layers.Softmax()
])
probability_model(x_test[:5])
```

Apptainer & GPUs

OUTPUT -
…stuff from finding NV devices ….
TensorFlow version: 2.11.0
Downloading data from https://storage.googleapis.com/tensorflow/tf-keras-datasets/mnist.npz
11490434/11490434 [==============================] - 1s 0us/step
2023-02-09 16:19:19.821484: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1613] Created device /job:localhost/replica:0/task:0/device:GPU:0 with 27060 MB memory: -> device: 0, name: Tesla V100-PCIE-32GB, pci bus id: 0000:17:00.0, compute capability: 7.0
2023-02-09 16:19:19.822409: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1613] Created device /job:localhost/replica:0/task:0/device:GPU:1 with 13779 MB memory: -> device: 1, name: Tesla T4, pci bus id: 0000:65:00.0, compute capability: 7.5
Epoch ⅕
2023-02-09 16:19:27.502094: I tensorflow/compiler/xla/service/service.cc:173] XLA service 0x7f3e84022ba0 initialized for platform CUDA (this does not guarantee that XLA will be used). Devices:
2023-02-09 16:19:27.502181: I tensorflow/compiler/xla/service/service.cc:181]   StreamExecutor device (0): Tesla V100-PCIE-32GB, Compute Capability 7.0
2023-02-09 16:19:27.502222: I tensorflow/compiler/xla/service/service.cc:181]   StreamExecutor device (1): Tesla T4, Compute Capability 7.5
2023-02-09 16:19:27.655725: I tensorflow/compiler/mlir/tensorflow/utils/dump_mlir_util.cc:268] disabling MLIR crash reproducer, set env var `MLIR_CRASH_REPRODUCER_DIRECTORY` to enable.
2023-02-09 16:19:29.277989: I tensorflow/compiler/jit/xla_compilation_cache.cc:477] Compiled cluster using XLA! This line is logged at most once for the lifetime of the process.
1875/1875 [==============================] - 8s 3ms/step - loss: 0.3024 - accuracy: 0.9112
Epoch ⅖
1875/1875 [==============================] - 6s 3ms/step - loss: 0.1465 - accuracy: 0.9573
Epoch ⅗
1875/1875 [==============================] - 4s 2ms/step - loss: 0.1113 - accuracy: 0.9662
Epoch ⅘
1875/1875 [==============================] - 5s 3ms/step - loss: 0.0901 - accuracy: 0.9718
Epoch 5/5
1875/1875 [==============================] - 6s 3ms/step - loss: 0.0759 - accuracy: 0.9766
313/313 - 1s - loss: 0.0813 - accuracy: 0.9760 - 645ms/epoch - 2ms/step

- Looks good - oh wait … none of the function evaluations show up in the output.

Apptainer & GPUs

- Python evaluations are NOT standard out. You want your results? Be sure to write them (or verify that they go to standard out)

Any python evaluation/function that outputs, throw it into an f.write

```
from tensorflow.python.client import device_lib
print(device_lib.list_local_devices())
import tensorflow as tf
print("TensorFlow version:", tf.__version__)
mnist = tf.keras.datasets.mnist

(x_train, y_train), (x_test, y_test) = mnist.load_data()
x_train, x_test = x_train / 255.0, x_test / 255.0
model = tf.keras.models.Sequential([
  tf.keras.layers.Flatten(input_shape=(28, 28)),
  tf.keras.layers.Dense(128, activation='relu'),
  tf.keras.layers.Dropout(0.2),
  tf.keras.layers.Dense(10)
])
predictions = model(x_train[:1]).numpy()
f = open('results.txt','w')
f.write(str(predictions) + '\n')
f.write(str(tf.nn.softmax(predictions).numpy()) + '\n')
loss_fn = tf.keras.losses.SparseCategoricalCrossentropy(from_logits=True)
f.write(str(loss_fn(y_train[:1], predictions).numpy()) + '\n')
model.compile(optimizer='adam',
              loss=loss_fn,
              metrics=['accuracy'])
f.write(str(model.evaluate(x_test,  y_test, verbose=2)) + '\n')
probability_model = tf.keras.Sequential([
  model,
  tf.keras.layers.Softmax()
])
f.write(str(probability_model(x_test[:5])) + '\n')
```

\n = newline (you probably knew that)

Here- I'm saying - open results.txt for writing

Skeptical cat is saying - "You're not labeling your output! It's garbage! Put in a f.write("Predictions!! %d\r\n") or whatever before every python evaluation! Imbecile!"
But maybe Skeptical cat doesn't realize I want to take the 'unadulterated' output and process through another program that would prefer not to have labels like "Predictions"?

Apptainer & GPUs

```
-bash-4.2$ more results.txt
[[-0.6788503   0.08507155  0.7489541  -0.3592714  -0.4191291   0.3637312
   0.15091619  0.44977978  0.41373825  0.18217495]]
[[0.04244909 0.09112456 0.17699295 0.05843321 0.05503815 0.12040813
  0.09732657 0.13122791 0.12658247 0.10041693]]
2.1168683
[2.3465797901153564, 0.08789999783039093]
tf.Tensor(
[[0.05063404 0.07061377 0.17750613 0.07071802 0.09076004 0.10206965
  0.13977249 0.08153952 0.09993464 0.11645163]
 [0.04648628 0.08442134 0.07763657 0.08092945 0.08309506 0.12882507
  0.19512239 0.10946266 0.11590897 0.07811217]
 [0.09442651 0.08400892 0.11063591 0.086678   0.09030239 0.09628462
  0.10558278 0.12173646 0.0983725  0.11197192]
 [0.04697128 0.08966808 0.14622916 0.03771305 0.04190792 0.08916441
  0.11697701 0.16301493 0.11301447 0.15533967]
 [0.08090983 0.05662173 0.11566644 0.11236666 0.06174224 0.15317099
  0.16894276 0.09333923 0.08112669 0.07611344]], shape=(5, 10), dtype=float32)
```

17 sig figs… useful… if you're measuring the diameter of a proton \s

- Voila. Yup. Exactly what I expected. Uh huh. Sure. Well- they are results, whether they mean anything is a different story.

Downloadable images

Especially for GPUs, there are some prebuilt images which are easy to work with

https://catalog.ngc.nvidia.com/ and, for example, if you search on Gromacs, you get

https://catalog.ngc.nvidia.com/orgs/hpc/containers/gromacs which has a docker image you can download(!!), as well as some instructions.

apptainer pull gromacs-2022.3.sif docker://nvcr.io/hpc/gromacs:2022.3

and then you can do your usual with your 'gromacs-2022.3.sif' file

cat runfile
/usr/local/gromacs/avx2_256/bin/gmx mdrun -ntomp 8 -ntmpi 4 -s benchRIB.tpr -nsteps 400

apptainer run --nv gromacs_2022.3.sif < runfile

Will run your gromacs job for ‘benchRIB’.

However…..

Security (or beware!)

- Yeah- be careful about any Docker images you find on the internet. It does not take too much imagination to create a Docker image called
  “Generate my Physics Thesis with ChatGPT”
  And, when you run it, it promptly deletes all your files.
- Trusted workflows, from trusted sources - a good start
- Apptainer uses private PGP keys to create a container signature, and the corresponding public key in order to verify the container signature. Verification of signed containers can be done at any time by a user and happens automatically in apptainer pull commands against Library API registries. The prevalence of PGP key servers, (like https://keys.openpgp.org/), make sharing and obtaining public keys for container verification relatively simple. Yup, sure, you’ll all do that.

Apptainer Instances

The subtitle to this slide is “How to impress a prospective employer to hire you at 6 figures”

- Instances are running containers waiting for interaction
- IMHO - these are not suitable for the clusters
- “Instances allow you to run containers as background processes. This can be useful for running services such as web servers or databases.”
- I only mention them because they will give you a feel for a cousin cluster called Nautilus that uses Kubernetes. If you say the word “Kubernetes” in a job interview, and mention “instances”, and how much you like containers, you’ll probably get the job.
- https://portal.nrp-nautilus.io/

Making your own Containers

Caveat: this is old for Singularity

- The Workflow – Step 1 – Build a linux VM so you can be root
  - Download and install a Virtual Machine application (I chose VirtualBox)
  - For pod.cnsi.ucsb.edu, build a CentOS 7 virtual machine
    - Choose your HD size so that it can accommodate your OS *and* your singularity images that you will create (i.e. 20GBs or so)
    - IchoseCentOS-7-x86_64-Everything-1804.isoasthebase
      - My favorite mirror is http://mirrors.oit.uci.edu/centos/7/isos/x86_64/
      - Remember that you want to install the Development Tools (Compute Node has it on the left)
    - Then we'll download and build singularity as we'll be root on our own little linux machine.
    - And then you can build singularity images to fit your exact needs. Once you've tested your workflow, you can copy those images to pod.cnsi.ucsb.edu and create jobs for them to run.

virtualbox.org

VirtualBox

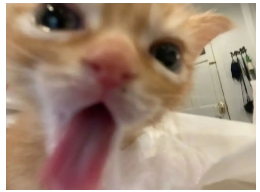
Login Preferences

Download VirtualBox

- About
- Screenshots
- Downloads
- Documentation
  - End-user docs
  - Technical docs
- Contribute
- Community

Here you will find links to VirtualBox binaries and its source code.

VirtualBox binaries



By downloading, you agree to the terms and conditions of the respective license.

If you're looking for the latest VirtualBox 5.1 packages, see VirtualBox 5.1 builds. Consider upgrading.

VirtualBox 5.2.20 platform packages

- Windows hosts
- OS X hosts
- Linux distributions
- Solaris hosts

The binaries are released under the terms of the GPL version 2.

See the changelog for what has changed.

You might want to compare the checksums to verify the integrity of downloaded packages. *The SHA256 checksums should be favored as the MD5 algorithm must be treated as insecure!*

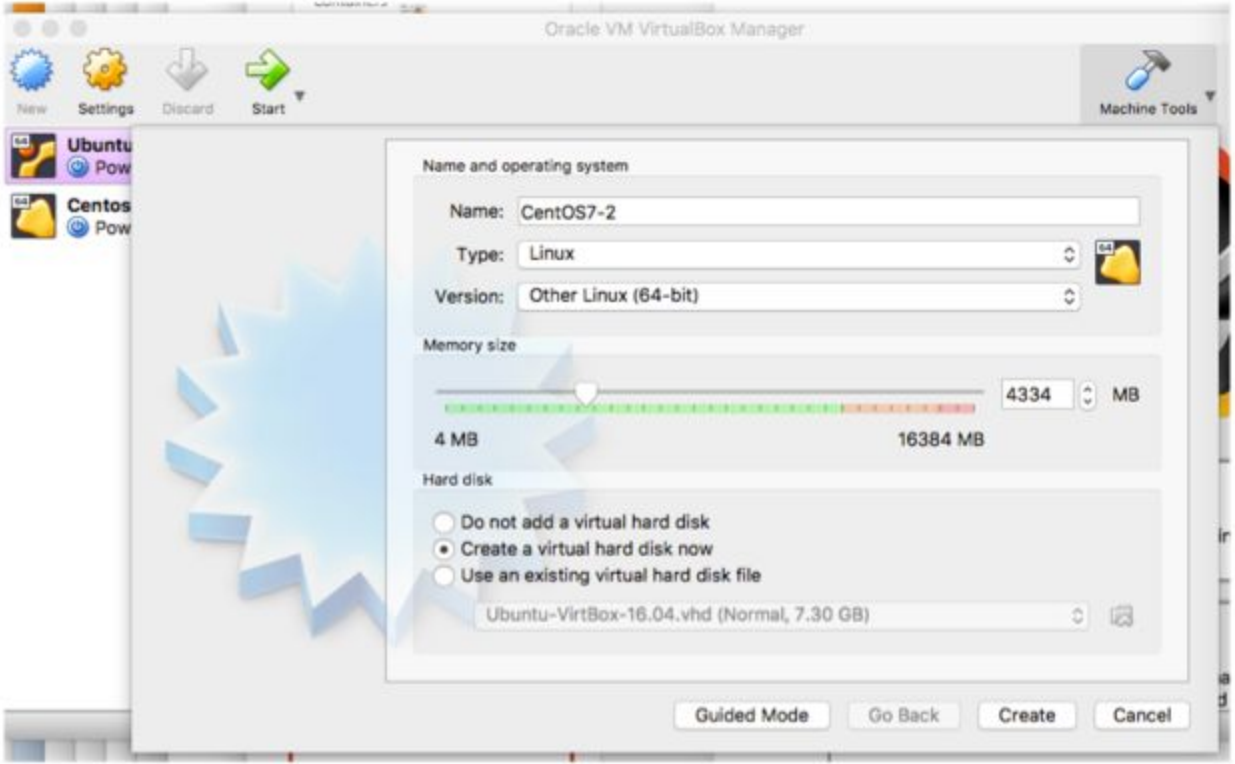
- SHA256 checksums, MD5 checksums

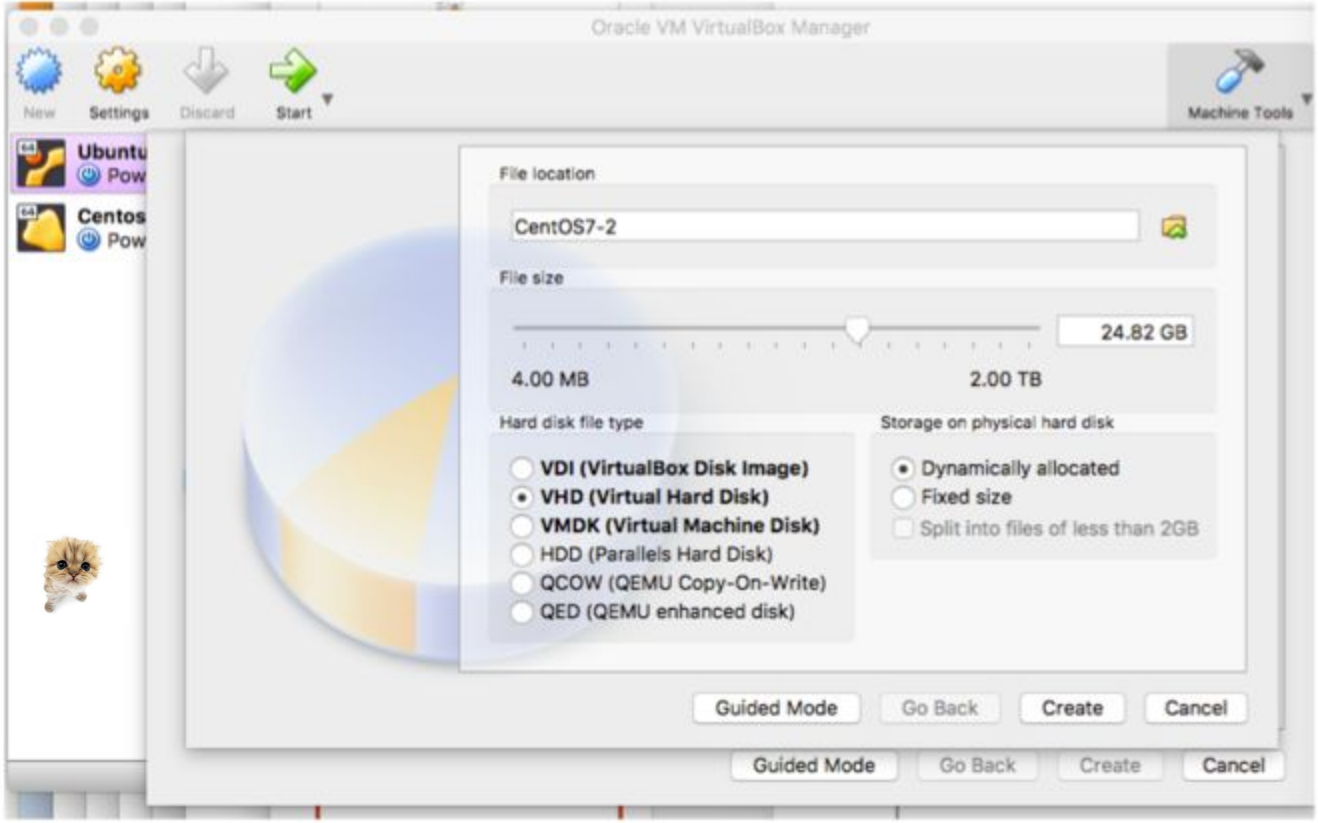
Note: After upgrading VirtualBox it is recommended to upgrade the guest additions as well.

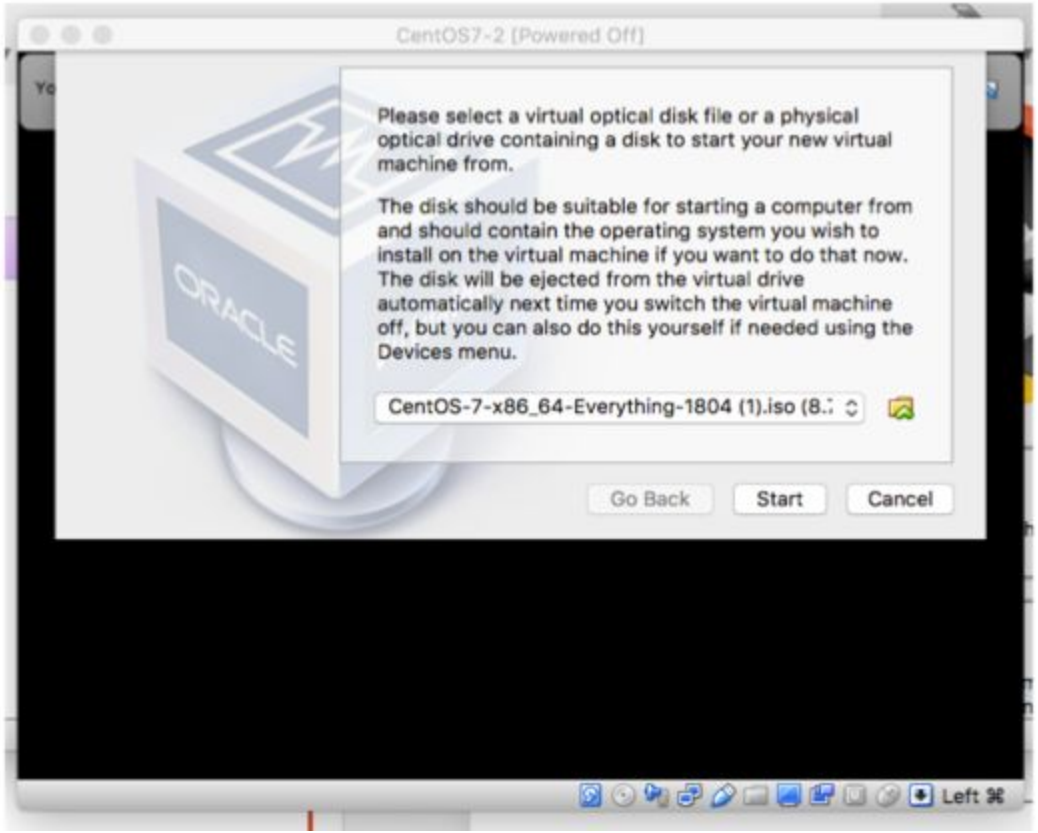
VirtualBox 5.2.20 Oracle VM VirtualBox Extension Pack

- All supported platforms

Support for USB 2.0 and USB 3.0 devices, VirtualBox RDP, disk encryption, NVMe and PXE boot for Intel cards. See this chapter from the User Manual for an introduction to this Extension Pack. The Extension Pack binaries are released under the VirtualBox Personal Use and Evaluation License (PUEL). *Please install the same version extension pack as your installed version of VirtualBox.*


Oracle VM VirtualBox Manager
New
Settings
Discard
Start
Machine Tools
Ubuntu
Pow
Centos
Pow
Name and operating system
Name: CentOS7-2
Type: Linux
Version: Other Linux (64-bit)
Memory size
4334
MB
4 MB
16384 MB
Hard disk
Do not add a virtual hard disk
Create a virtual hard disk now
Use an existing virtual hard disk file
Ubuntu-VirtBox-16.04.vhd (Normal, 7.30 GB)
Guided Mode
Go Back
Create
Cancel


Oracle VM VirtualBox Manager
New
Settings
Discard
Start
Machine Tools
Ubuntu
Pow
Centos
Pow
File location
CentOS7-2
File size
24.82 GB
4.00 MB
2.00 TB
Hard disk file type
VDI (VirtualBox Disk Image)
VHD (Virtual Hard Disk)
VMDK (Virtual Machine Disk)
HDD (Parallels Hard Disk)
QCOW (QEMU Copy-On-Write)
QED (QEMU enhanced disk)
Storage on physical hard disk
Dynamically allocated
Fixed size
Split into files of less than 2GB
Guided Mode
Go Back
Create
Cancel
Guided Mode
Go Back
Create
Cancel


CentOS7-2 [Powered Off]
Please select a virtual optical disk file or a physical optical drive containing a disk to start your new virtual machine from.
The disk should be suitable for starting a computer from and should contain the operating system you wish to install on the virtual machine if you want to do that now. The disk will be ejected from the virtual drive automatically next time you switch the virtual machine off, but you can also do this yourself if needed using the Devices menu.
CentOS-7-x86_64-Everything-1804 (1).iso (8.
Go Back
Start
Cancel
Left ⌘

CentOS7-2 (Running)

SOFTWARE SELECTION

Done

CENTOS 7 INSTALLATION

us

Help!

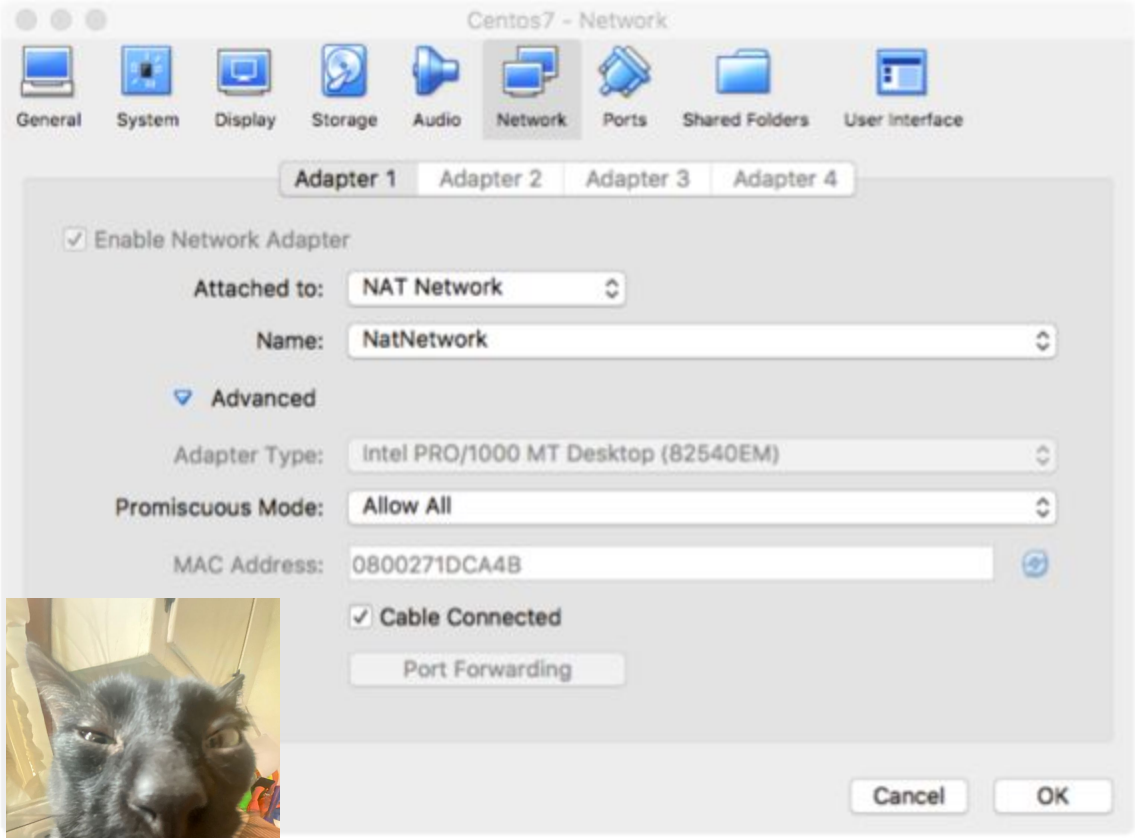
Base Environment

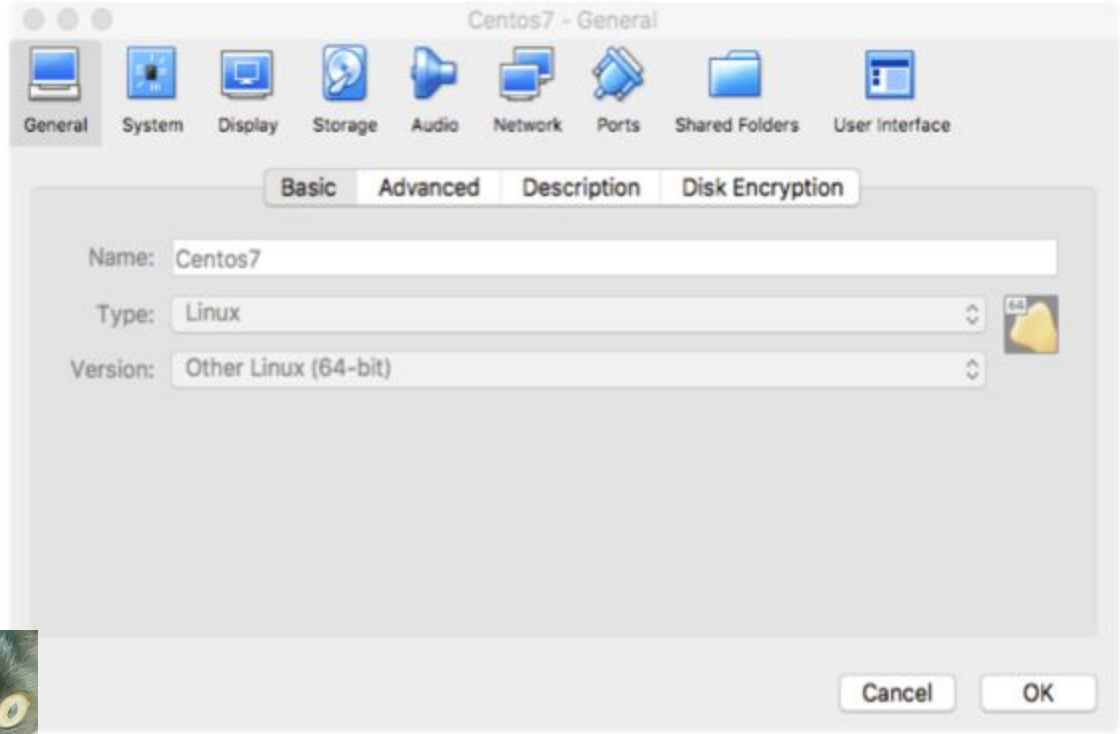
- **Minimal Install**
  Basic functionality.
- **Compute Node**
  Installation for performing computation and processing.
- **Infrastructure Server**
  Server for operating network infrastructure services.
- **File and Print Server**
  File, print, and storage server for enterprises.
- **Basic Web Server**
  Server for serving static and dynamic internet content.
- **Virtualization Host**
  Minimal virtualization host.
- **Server with GUI**
  Server for operating network infrastructure services, with a GUI.
- **GNOME Desktop**
  GNOME is a highly intuitive and user friendly desktop environment.
- **KDE Plasma Workspaces**
  The KDE Plasma Workspaces, a highly-configurable graphical user interface which includes a panel, desktop, system icons and desktop widgets, and many powerful KDE applications.
- **Development and Creative Workstation**
  Workstation for software, hardware, graphics, or content development.

Add-Ons for Selected Environment

- **Debugging Tools**
  Tools for debugging misbehaving applications and diagnosing performance problems.
- **Directory Client**
  Clients for integration into a network managed by a directory service.
- **Guest Agents**
  Agents used when running under a hypervisor.
- **Hardware Monitoring Utilities**
  A set of tools to monitor server hardware.
- **Infiniband Support**
  Software designed for supporting clustering and grid connectivity using RDMA-based InfiniBand and iWARP fabrics.
- **Network File System Client**
  Enables the system to attach to network storage.
- **Performance Tools**
  Tools for diagnosing system and application-level performance problems.
- **Remote Management for Linux**
  Remote management interface for CentOS Linux, including OpenLMI and SNMP.
- **Compatibility Libraries**
  Compatibility libraries for applications built on previous versions of CentOS Linux.
- **Development Tools**
  A basic development environment.
- **Security Tools**
  Security tools for integrity and trust verification.
- **Smart Card Support**
  Support for using smart card authentication.
- **System Administration Tools**
  Utilities useful in system administration.

Left ⌘


Centos7 - Network
General
System
Display
Storage
Audio
Network
Ports
Shared Folders
User Interface
Adapter 1
Adapter 2
Adapter 3
Adapter 4
Enable Network Adapter
Attached to:
NAT Network
Name:
NatNetwork
Advanced
Adapter Type:
Intel PRO/1000 MT Desktop (82540EM)
Promiscuous Mode:
Allow All
MAC Address:
0800271DCA4B
Cable Connected
Port Forwarding
Cancel
OK


Centos7 - General
General
System
Display
Storage
Audio
Network
Ports
Shared Folders
User Interface
Basic
Advanced
Description
Disk Encryption
Name:
Centos7
Type:
Linux
Version:
Other Linux (64-bit)
Cancel
OK

Making your own Containers

- The Workflow – Step 2 – Getting and Building Singularity / Apptainer
  - Start your VM from VirtualBox, login as root
  - https://github.com/sylabs/singularity/releases - the .tar.gz are fine
    - wget https://github.com/sylabs/singularity/releases/download/2.5.2/singularity-2.5.2.tar.gz
    - gunzip that file, untar that file
    - cdsingularity-2.5.2
    - ./configure –prefix=/singularity (prefix not necessary) Note if configure fails with missing packages – you might need to yum install somepackagelikegcc
    - make - if there are no errors....
    - make install
    - yum install epel-release , yum install debootstrap
- Voila – you now have singularity in your VM and can create singularity / apptainer containers

Making your own Singularity Containers

- The Workflow – Step 3 – Creating an Ubuntu container

- Build an empty container

  - export PATH=$PATH:/singularity/bin
  - singularitycreateubuntu.img
  - singularityimage.expand–size4000ubuntu.img
  - singularitybuildubuntu.img createdeb.def wherecreatedeb.def:

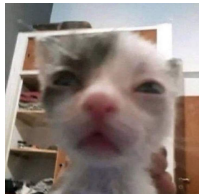
    BootStrap: debootstrap
    DistType: Debian
    MirrorURL: http://us.archive.ubuntu.com/ubuntu

    OSVersion: xenial
    %runscript
    apt-get install python

  - singularity shell ubuntu.img ← you're now in the container (--writable)
  - apt-get install python sudo ← and anything else you want to install (might need sudo for other apt-gets like sudo apt-get install somepackageoranother – so you need sudo)
  - Exit ← gets you out the container back into CentOS 7

Next Steps

- Now that you have a container- customize it to work with your workflow. Install whatever packages you need.
- When you use a container on the clusters, it automatically mounts your home directory.
- The container sees all of the system's memory and CPUs, but none of the other filesystems/directories unless you explicitly mount them – and then they're generally readonly unless it's /scratch.
  • singularityshell-B/scratch:/mnt/sw/singularity/SingularityImages-knot/ubuntu_croco.img Here, the /scratch directory is mounted in your container at /mnt.
- From your CentOS 7 install, scp myubuntu.img username@pod.cnsi.ucsb.edu
- Note that once your image is on the clusters, it is immutable (unless you ask us to alter something)



- Example job submission file on pod.cnsi.ucsb.edu – test-croco.job

```
#!/bin/bash -l
#Serial (1 core on one node) job…
#SBATCH --nodes=1 --ntasks-per-node=1
cd $SLURM_SUBMIT_DIR
source .bashrc
singularity exec -B /scratch:/mnt /sw/singularity/SingularityImages-knot/ubuntu_croco.img /home/fuz/test-croco.in
```

- Example run file for the container – test-croco.in

```
export PATH=/home/fuz/anaconda2/bin:$PATH apt list --installed
echo ""
echo "Which python am I using:"
which python
echo ""
Echo "Determine whether a number is prime or not" python primeornot.py
```

- Submit the job
  - sbatch test-croco.job