Using Containers on the Cannon Cluster : Singularity

Objectives

- What are containers and why we care? (overview)
- Singularity container system
- How to run Singularity containers on Cannon:
  - running simple containers
  - pulling from docker registry or sylab library
  - Using GPUs
- How to build your own containers
  - docker
  - bind mount
- How do I get help?

What problems are we trying to solve?

Deploying Applications:

Building software is often a complicated business, particularly on HPC and other multi-tenant systems:

- HPC clusters have typically very specialized software stacks which might not adapt well to general purpose applications.
- OS installations are streamlined.
  Some applications might need dependencies that are not readily available and complex to build from source.
- End users use Ubuntu or Arch, cluster typically use RHEL, or SLES, or other specialized OS.
  (... “>$ sudo apt-get install “ will not work)

What problems are we trying to solve?

Portability and Reproducibility:

- Running applications on multiple systems typically needs replicating the installations multiple times making it hard to keep consistency.
- It would be useful to publish the exact application used to run a calculation for reproducibility or documentation purpose.
- As a user can I minimize the part of the software stack I have no control on, to maximize reproducibility without sacrificing performance?

What problems are we trying to solve?

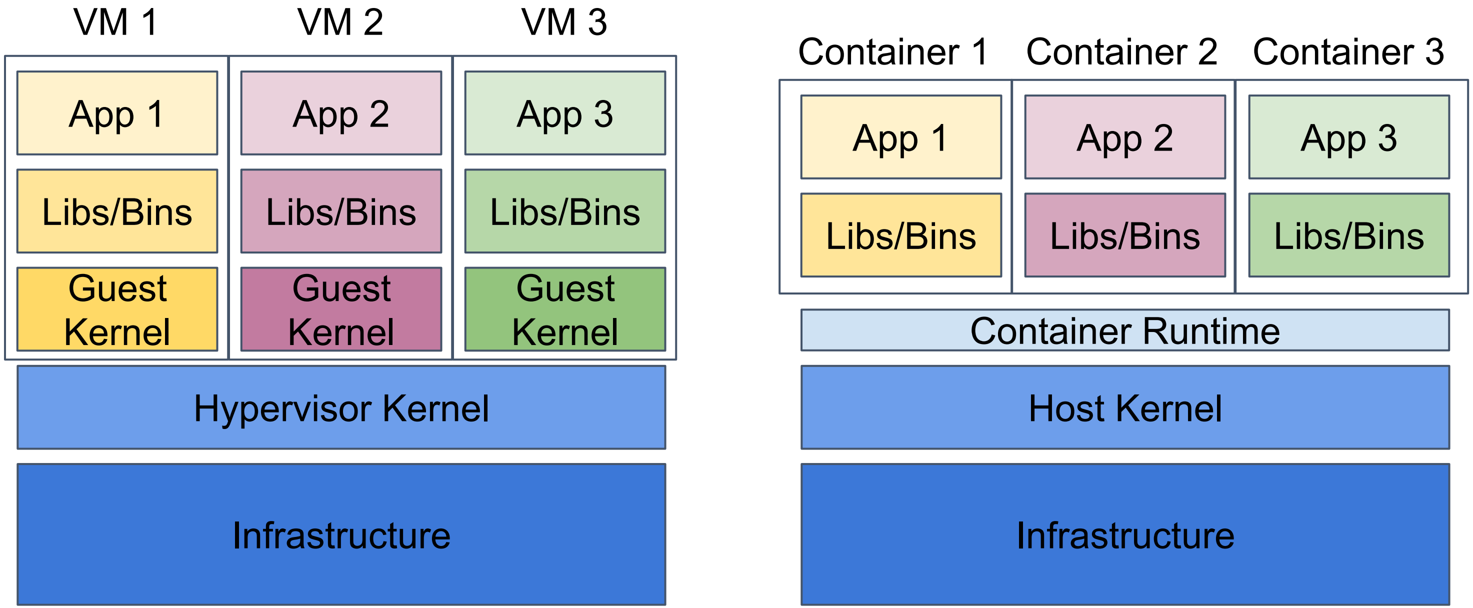
Resource Contention and Security:

- Tasks on a normal OS float between cores and memory space.
- Want to set a cap on usage for multiple tenants.
- Ensure users cannot see other users applications and satck

Types of Containers

- cgroups
- python/conda environment
- Docker-like containers
- Virtual Machine (VM)

VMs or Containers



VMs:
hardware virtualization + OS

Containers:
User defined software stack

Containers: easi"er" software deployment

Containers provide a potential solution…. or at the very least can help.

- Easier software deployment:
  Users can leverage on installation tools that do not need to be available natively on the runtime host
  (e.g. package managers of various linux distributions).
- Software can be built on a platform different from the exec hosts.
- they package in one single object all necessary dependencies.
- easy to publish and sign
- they are portable **
  - … provided you run on a compatible architecture)
  - access to special hardware needs special libraries also inside the container , which at the moment limits portability

Types of Containers

docker

Linux LXC

OpenVZ
Linux Containers

podman

rkt

Charliecloud

SHIFTER

General purpose / microservice Oriented.

HPC Oriented :

- Compatible with WLM
- No privilege escalation needed

Singularity (https://www.sylabs.io)

Singularity provides a container runtime and an ecosystem for managing images that is suitable for multi-tenant systems and HPC environments.
Important aspects :

- no need to have elevated privileges at runtime, although root privileges are needed to build the images.
- each applications will have its own container
- containers are not fully isolated (e.g. host network is available)
- users have the same uid and gid when running an application
- containers can be executed from local image files, or pulling images from a docker registry, a singularity hub or from sylab libraries (see https://cloud.sylabs.io … N.B. service is still in alpha)

For basic usage refer to
https://www.rc.fas.harvard.edu/resources/documentation/software/singularity-on-odyssey/
https://www.sylabs.io/docs/

Example : running from a docker registry

Running tensorflow on a cpu node

```
login-node      ] >$ srun  --pty --mem=4000 -p test -N 1 -t 60  /bin/bash
compute-node ] >$ cd $SCRATCH/your_lab/your_user/
compute-node ] >$ git clone https://github.com/tensorflow/models.git
compute-node ] >$  singularity exec docker://tensorflow/tensorflow:latest-py3 python \
                  ./models/tutorials/image/mnist/convolutional.py
```

Running tensorflow on a gpu node

```
login-node      ] >$ srun  --pty --mem=4000 -p gpu --gres=gpu  -N 1 -t 60  /bin/bash
compute-node ] >$ cd $SCRATCH/your_lab/your_user/
compute-node ] >$ git clone https://github.com/tensorflow/models.git
compute-node ] >$  singularity exec  --nv docker://tensorflow/tensorflow:latest-gpu-py3 python \
                  ./models/tutorials/image/mnist/convolutional.py
```

Example : pulling images from a repositories

pulling from docker

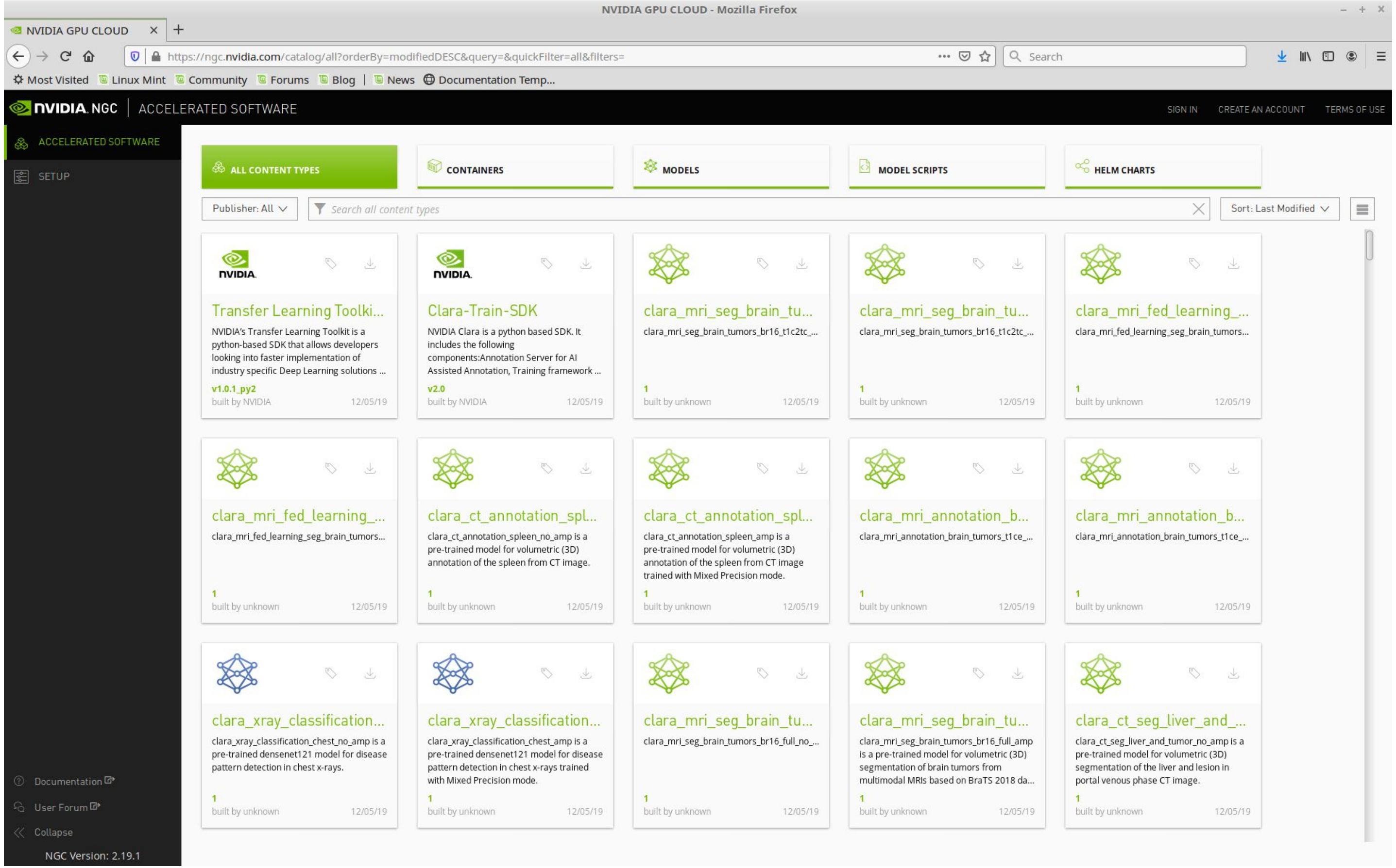
```
login-node      ] >$ srun  --pty --mem=4000 -p test -N 1 -t 60  /bin/bash
compute-node ] >$ cd $SCRATCH/your_lab/your_user/
compute-node ] >$ singularity pull docker://tensorflow/tensorflow:latest-gpu-py3
compute-node ] >$
```

pulling from shub

```
login-node      ] >$ srun  --pty --mem=4000   -p test -N 1 -t 60  /bin/bash
compute-node ] >$ cd $SCRATCH/your_lab/your_user/
compute-node ] >$ singularity pull shub://vsoch/hello-world
```

pulling from library

```
login-node      ] >$ srun  --pty --mem=4000   -p test -N 1 -t 60  /bin/bash
compute-node ] >$ cd $SCRATCH/your_lab/your_user/
compute-node ] >$ singularity pull mylolcow.sif   \
                          library://francesco/examples/lolcow_odyssey:latest
```


NVIDIA GPU CLOUD - Mozilla Firefox
NVIDIA GPU CLOUD
https://ngc.nvidia.com/catalog/all?orderBy=modifiedDESC&query=&quickFilter=all&filters=
Search
Most Visited
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Forums
Blog
News
Documentation Temp...
NVIDIA NGC
ACCELERATED SOFTWARE
SIGN IN
CREATE AN ACCOUNT
TERMS OF USE
ACCELERATED SOFTWARE
SETUP
ALL CONTENT TYPES
CONTAINERS
MODELS
MODEL SCRIPTS
HELM CHARTS
Publisher: All
Search all content types
Sort: Last Modified
Transfer Learning Toolki...
NVIDIA's Transfer Learning Toolkit is a python-based SDK that allows developers looking into faster implementation of industry specific Deep Learning solutions ...
v1.0.1_py2
built by NVIDIA
12/05/19
Clara-Train-SDK
NVIDIA Clara is a python based SDK. It includes the following components:Annotation Server for AI Assisted Annotation, Training framework ...
v2.0
built by NVIDIA
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clara_ct_annotation_spl...
clara_ct_annotation_spleen_no_amp is a pre-trained model for volumetric (3D) annotation of the spleen from CT image.
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clara_ct_annotation_spl...
clara_ct_annotation_spleen_amp is a pre-trained model for volumetric (3D) annotation of the spleen from CT image trained with Mixed Precision mode.
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clara_mri_annotation_b...
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clara_mri_annotation_b...
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clara_xray_classification...
clara_xray_classification_chest_no_amp is a pre-trained densenet121 model for disease pattern detection in chest x-rays.
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clara_xray_classification...
clara_xray_classification_chest_amp is a pre-trained densenet121 model for disease pattern detection in chest x-rays trained with Mixed Precision mode.
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clara_mri_seg_brain_tu...
clara_mri_seg_brain_tumors_br16_full_amp is a pre-trained model for volumetric (3D) segmentation of brain tumors from multimodal MRIs based on BraTS 2018 da...
1
built by unknown
12/05/19
clara_ct_seg_liver_and_...
clara_ct_seg_liver_and_tumor_no_amp is a pre-trained model for volumetric (3D) segmentation of the liver and lesion in portal venous phase CT image.
1
built by unknown
12/05/19
Documentation
User Forum
Collapse
NGC Version: 2.19.1

Example : running from a local image

```
## Running matlab

login-node      ] >$ srun  --pty --mem=4000 -p test -N 1 -t 60  /bin/bash
compute-node ] >$ cd $SCRATCH/your_lab/your_user/
compute-node ] >$ myimage=/n/helmod/apps/centos7/Singularity/matlab/matlab-2018-el7-7.4.1708.img
compute-node ] >$  singularity exec $myimage matlab -nodesktop -nosplash
```

RC Portal - Mozilla Firefox

RC Portal

https://portal.rc.fas.harvard.edu/p3/build-reports/

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Singularity 3

Cactus

Cactus is a reference-free whole-genome multiple alignment program

cactus 2019-11-29

Please see detailed instructions for the use of this cactus image on the FAS Informatics website.

To activate this build:

```
singularity exec --cleanenv /n/singularity_images/informatics/cactus/cactus:2019-11-29.sif --binariesMode local jobStore "${SEQFILE}" "${OUTPUTHAL}"
```

Cell Ranger ATAC

Cell Ranger ATAC is a set of analysis pipelines that process Chromium Single Cell ATAC data

Running cluster job

```
#!/bin/bash
#SBATCH -n 1
#SBATCH -p test
#SBATCH --mem=4G
#SBATCH -t 1-00:00:00

singularity run my_image.sif
```

or

```
singularity exec my_image.sif mycommand
```

Build your first container

Container images can be built using a file that specifies the recipe.

For example :

```
>$ cat Singularity
BootStrap: debootstrap
OSVersion: trusty
MirrorURL: http://us.archive.ubuntu.com/ubuntu/

%runscript
    echo "This is what happens when you run the container..."

%post
    echo "Hello from inside the container"
    sed -i 's/$/ universe/' /etc/apt/sources.list
    apt-get update
    apt-get -y install vim
    apt-get clean
```

complete description of the def files at

https://www.sylabs.io/guides/3.4/user-guide/definition_files.html

Build your first container

Once I have my singularity file I have three options to build my image:

1. Build Locally

To do this you need to be on your own development environment where you have admin privileges.

```
mycomputer ]> sudo /usr/local/bin/singularity build some_imagename.sif  Singularity.def
```

2. Build remotely

You can do it on Cannon, but you need to have an account on https://cloud.sylabs.io , get a token and store it in ~/.singularity/sylabs-token

```
login-node      ] >$ srun  --pty --mem=4000   -p test -N 1 -t 60  /bin/bash
compute-node ] >$ cd $SCRATCH/your_lab/your_user/
compute-node ] >$ singularity build --remote  some_imagename.sif Singularity.def
```

this will create your def file, build the image and download it to the local folder.

Build your first container (3): Docker

- You can build an image in Docker on your local machine
  - Has the advantage of quicker iteration

- Export to dockerhub or use docker2singularity (https://github.com/singularityhub/docker2singularity)

- Pull image to cluster in singularity, or scp it and use.

Bind Mount

- By default all directories in the Singularity image are read only.
  - **Note:** When building from Docker, sometimes Docker expects something to be writable that may not be in Singularity.

- In addition system directories are not available, only those defined in the Singularity image.

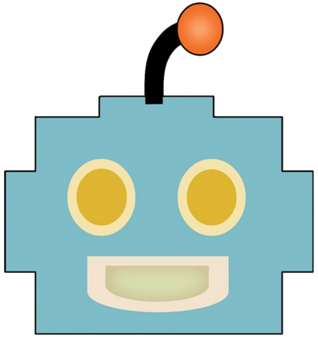
- You can bind external mounts into singularity using the -B option
  - -B hostdir:containerdir
  - -B hostdir <- Maps it to same path inside the container

```
singularity exec -B /scratch:/var/log ls /var/log
```

- On Cannon, we automatically map /n, /net, and /scratch into the image using bind mount.

Request Help - Resources

- https://rc.fas.harvard.edu/resources/support/
  - Documentation
    - https://rc.fas.harvard.edu/resources/documentation/
  - Portal
    - http://portal.rc.fas.harvard.edu/rcrt/submit_ticket
  - Email
    - rchelp@rc.fas.harvard.edu
  - Office Hours
    - Wednesday noon-3pm 38 Oxford - 206
  - Training
    - https://www.rc.fas.harvard.edu/upcoming-training/



- RC Staff are here to help you and your colleagues effectively and efficiently use Cannon resources to expedite your research endeavors.
- Please acknowledge our efforts:
  - "The computations in this paper were run on the FASRC Cannon cluster supported by the FAS Division of Science Research Computing Group at Harvard University."
  - https://rc.fas.harvard.edu/about/attribution/