University of Colorado **Anschutz Medical Campus**

Container workshop

By Kevin Fotso

Where are the container software?

There are two ways:

- Apptainer, which is installed at a system level on any compute partition (e.g. acompile, atesting, amilan etc…) .

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/usr/bin/apptainer
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- Singularity, which needs to be loaded using LMOD at a system level on any compute partition (e.g. acompile, atesting, amilan etc…) .

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- Apptainer, which is installed at a system level on any compute partition (e.g. acompile, atesting, amilan etc…) .

```
~]$  which apptainer
/usr/bin/apptainer
```

- singularity, which needs to be loaded using at a system level on any compute partition (e.g. acompile, atesting, amilan etc…) .

```
~]$  module avail singularity

singularity/3.6.4 (D)        singularity/3.7.4

~]$  module load singularity

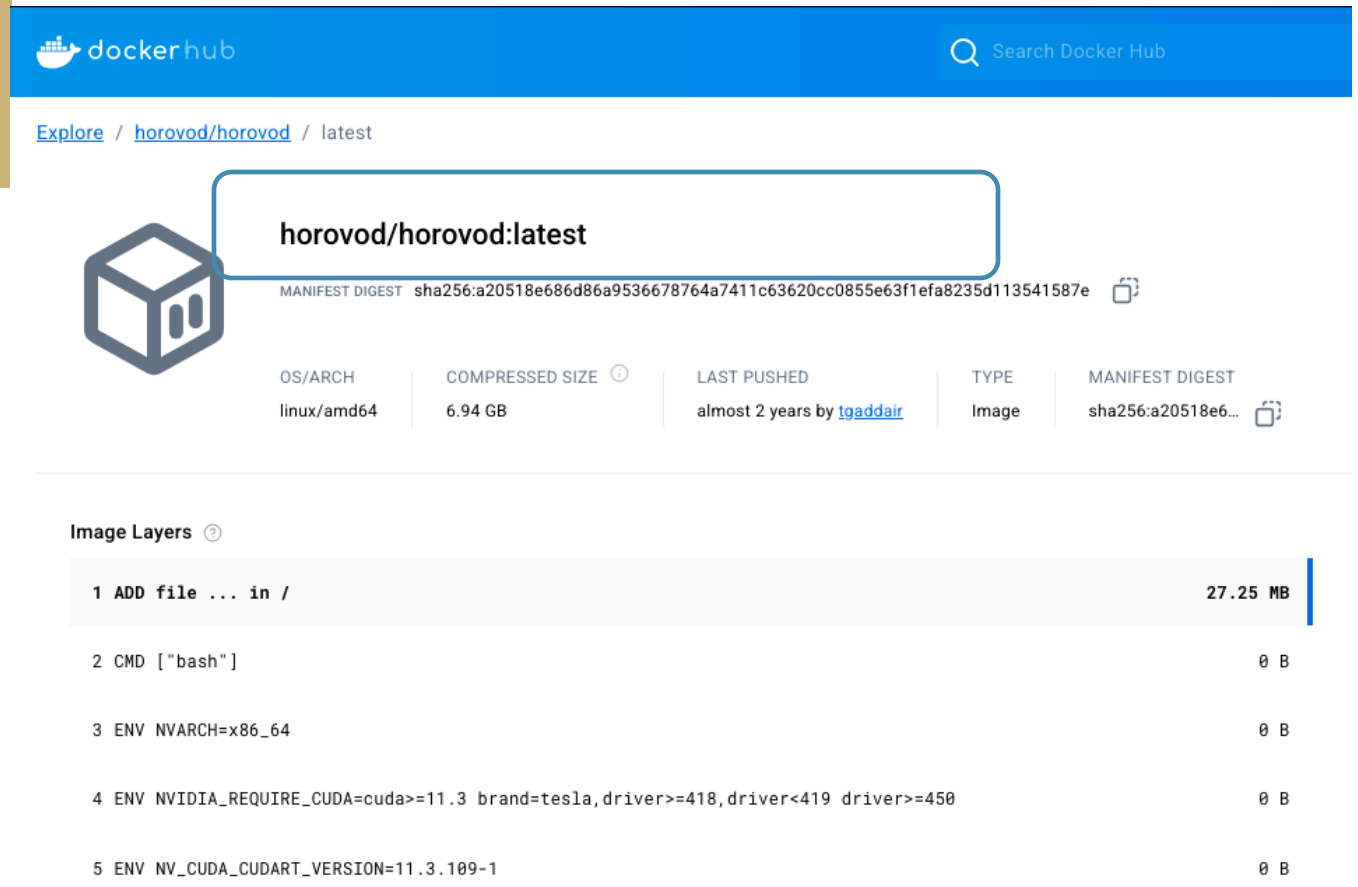
~]$  module list

Currently loaded modules:
1)  slurm/alpine 2) curc-quota/latest 3) StdEnv
4) singularity/3.6.4
```

What are apptainer vs singularity?

- They originally came from the same project called singularity under the Sylabs umbrella.
- A fork occurred in 2020 which eventually led to SingularityCE for Sylabs and apptainer under the Linux Foundation umbrella
  - Source: https://groups.google.com/a/lbl.gov/g/singularity/c/UbywVHXD_co/m/bGa8M4QAAQAJ
  - https://groups.google.com/a/lbl.gov/g/singularity/c/lRWR3vJGvks/m/bMvv9OfYBAAJ?pli=1

Let’s use a Docker container!



- Horovod allows to run distributed deep learning on multiple cpus, gpus and nodes.

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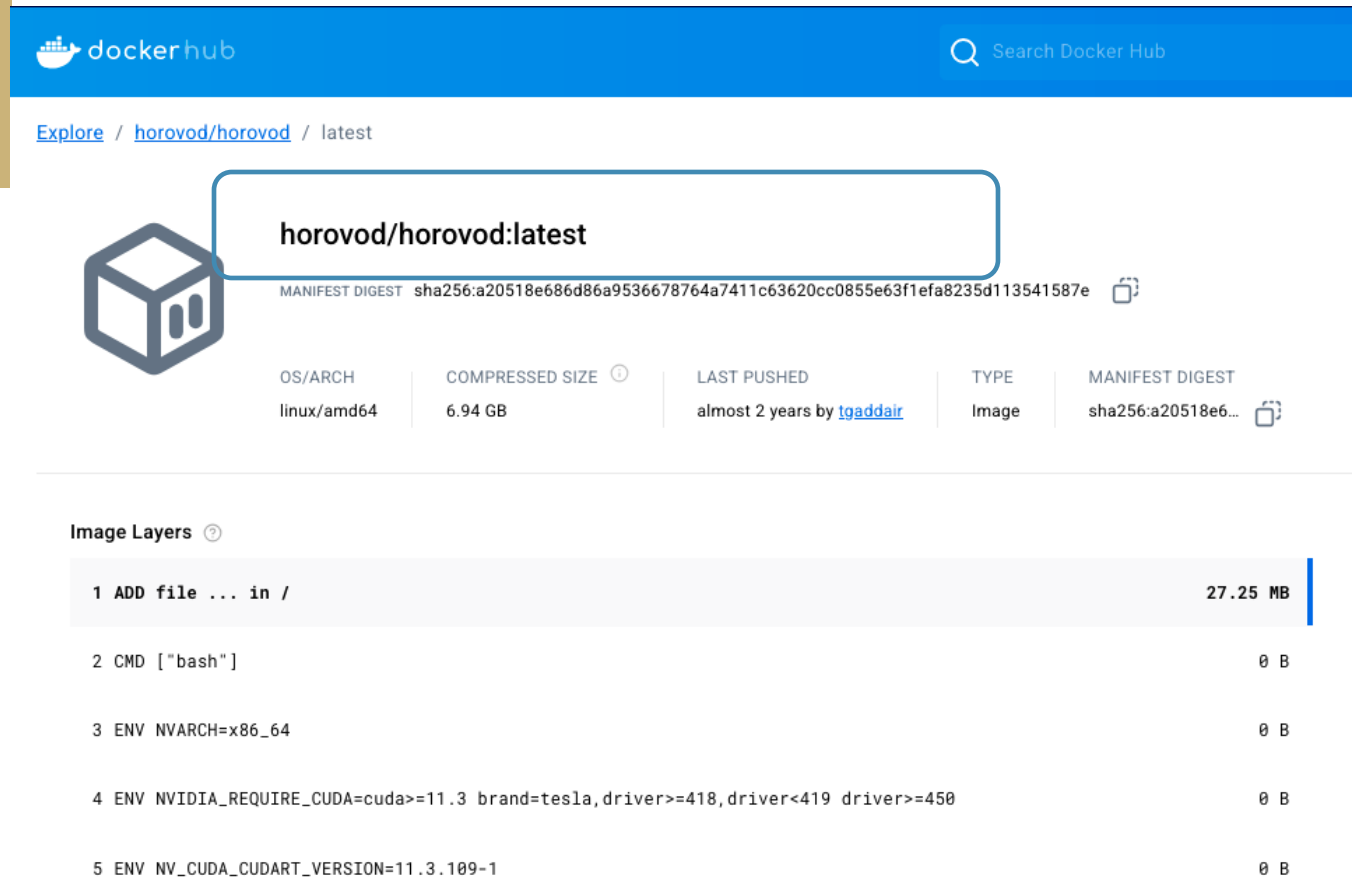
Source:

https://hub.docker.com/layers/horovod/horovod/latest/images/sha256-a20518e686d86a9536678764a7411c63620cc0855e63f1efa8235d113541587e?context=explore

Let’s use a Docker container!



- Horovod allows run distributed deep learning on multiple cpus, gpus and nodes.

- Please refer to our workshop here:

https://github.com/kf-cuanschutz/CU-Anschutz-HPC-documentation/blob/main/Workshops/Introduction_to_Horovod_102423_part1_official_v2.pdf

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Source:

https://hub.docker.com/layers/horovod/horovod/latest/images/sha256-a20518e686d86a9536678764a7411c63620cc0855e63f1efa8235d113541587e?context=explore

Let’s use a Docker container!

- We make sure to go to a compute node on Alpine

```
@login-ci1 ~]$ acompile –ntasks=4 –time=12:00:00

@c3cpu-a2-u32-2 ~]$
```

Let’s use a Docker container!

- We make sure to go to a compute node on Alpine

```
@login-ci1 ~]$ acompile –ntasks=4 –time=12:00:00

@c3cpu-a2-u32-2 ~]$
```

- Because the filesystem /tmp is small on Alpine, we probably want to export tmp directories to the scratch filesystem.

```
@c3cpu-a2-u32-2 ~]$ export ALPINE_SCRATCH=/gpfs/alpine1/scratch/$USER
@c3cpu-a2-u32-2 ~]$ export APPTAINER_TMPDIR=$ALPINE_SCRATCH/apptainer/tmp
@c3cpu-a2-u32-2 ~]$ export APPTAINER_TMPDIR=$ALPINE_SCRATCH/apptainer/cache
@c3cpu-a2-u32-2 ~]$ mkdir -pv $APPTAINER_TMPDIR $APPTAINER_TMPDIR
```

We convert the docker img into apptainer

- We use the build command, which works equally for apptainer or singularity.

```
@c3cpu-a2-u32-2 ~]$ apptainer build horovod.sif docker://horovod/horovod:latest
INFO: Starting build...
Copying blob 326d76058f67 skipped: already exists
Copying blob 846c0b181fff skipped: already exists
Copying blob 6fc9dd88827c skipped: already exists
```

We can also build a container image out of a def file

- We create what is called a definition file, which will create the necessary instructions to build the container image

This section helps to create the base OS I want.

```
Bootstrap: debootstrap
OSVersion: focal
MirrorURL: http://us.archive.ubuntu.com/ubuntu/
Include: apt
%labels
   Author Kevin Fotso
   Version v1.0.0
%files
   /home/fotsok/spliceAI/SpliceAI /NGS_tools/
%post
   # non-interactive debconf
   export DEBIAN_FRONTEND=noninteractive
DEBCONF_NONINTERACTIVE_SEEN=true
   # update apt
   apt-get update
   # install python3 and snakemake
   apt update
   apt install -y     wget \
            gfortran \
```

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To give some comments and select the package manager toolbox associated with the OS

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%files allow to copy files from the host system into the container during the build process.

```
Bootstrap: debootstrap
OSVersion: focal
MirrorURL: http://us.archive.ubuntu.com/ubuntu/
Include: apt
%labels
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   Version v1.0.0
%files
   /home/fotsok/spliceAI/SpliceAI /NGS_tools/
%post
   # non-interactive debconf
   export DEBIAN_FRONTEND=noninteractive
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```

This section allows to pass write config files, create new directories, variables.

Noninteractive is very suitable for automatic build and and to have zero interaction while installing.

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Include: apt
%labels
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   apt update
   apt install -y     wget \
            gfortran \
```

Here, I can install the packages

We can also build a container image out of a def file

- We create what is called a definition file, which will create the necessary instructions to build the container image

Here, I can export other environmental variables

```
%environment
export CONDA_PREFIX='/opt/software/conda'
export PATH='/opt/software/conda/bin':$PATH
export LD_LIBRARY_PATH=$CONDA_PREFIX/lib/python3.10/site-packages/nvidia/cudnn/lib:$CONDA_PREFIX/pkgs/cuda-nvcc-11.8.89-0/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=/opt/software/conda/lib:$LD_LIBRARY_PATH
%test
	echo $PATH
%runscript
	exec "$@"
```

We can also build a container image out of a def file

- We create what is called a definition file, which will create the necessary instructions to build the container image

```
%environment
export CONDA_PREFIX='/opt/software/conda'
export PATH='/opt/software/conda/bin':$PATH
export LD_LIBRARY_PATH=$CONDA_PREFIX/lib/python3.10/site-packages/nvidia/cudnn/lib:$CONDA_PREFIX/pkgs/cuda-nvcc-11.8.89-0/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=/opt/software/conda/lib:$LD_LIBRARY_PATH
%test
    echo $PATH
%runscript
    exec "$@"
```

It can be used to test the ENV at the end

e.g. if the binaries where downloaded properly or a software runs as expected in a testing ENV.

We can also build a container image out of a def file

- We create what is called a definition file, which will create the necessary instructions to build the container image

```
%environment
export CONDA_PREFIX='/opt/software/conda'
export PATH='/opt/software/conda/bin':$PATH
export LD_LIBRARY_PATH=$CONDA_PREFIX/lib/python3.10/site-
packages/nvidia/cudnn/lib:$CONDA_PREFIX/pkgs/cuda-nvcc-11.8.89-
0/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=/opt/software/conda/lib:$LD_LIBRARY_PATH
%test
	echo $PATH
%runscript
	exec "$@"
```

Contents are written to a file when the container is running.

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More information here:
https://apptainer.org/docs/user/main/definition_files.html

We can also build a container image out of a def file

- We run the build command out of the definition file.

```
@c3cpu-a2-u32-2 scripts]$ apptainer build splice_conda.img splice_conda.def
```

- Warning! You can only build a container that way on Alpine with apptainer and not singularity!

More information here:
https://curc.readthedocs.io/en/latest/software/containerization.html

Let’s submit a container application slurm script

- We run the build command out of the definition file.

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --partition=amilan
#SBATCH --time=03:00:00
#SBATCH --mem=100G
#SBATCH --job-name="rsem_prepare_and_run”
#SBATCH -o "rsem_star.%j.out”
#SBATCH -e "rsem_star.%j.err”
#SBATCH --account=amc-general
#SBATCH --qos=normal
```

Always request 1 node, unless you are using a distributed application

Let’s submit a container application slurm script

- We run the build command out of the definition file.

```
export ALPINE_SCRATCH=/gpfs/alpine1/scratch/$USERexport
APPTAINER_TMPDIR=$ALPINE_SCRATCH/apptainer/tmpexport
APPTAINER_CACHEDIR=$ALPINE_SCRATCH/apptainer/cache
mkdir -pv $APPTAINER_CACHEDIR $APPTAINER_TMPD
```

Always export tmp related
Directory variables to your scratch!
In case you are using **apptainer!**

Let’s submit a container application slurm script

- We run the build command out of the definition file.

```
export ALPINE_SCRATCH=/gpfs/alpine1/scratch/$USERexport
export SINGULARITY_TMPDIR=$ALPINE_SCRATCH/singularity/tmp
export SINGULARITY_CACHEDIR=$ALPINE_SCRATCH/singularity/cache
mkdir -pv $SINGULARITY_CACHEDIR $SINGULARITY_TMPDIR
```

In case you use **singularity** instead!

Let’s submit a container application slurm script

- You might need to bind some key directories or filesystems that you will export inside your container when running it.

```
export CONTAIN_DIR=/scratch/alpine/kfotso@xsede.org/Seq
cd ${CONTAIN_DIR}
input_dir="${PWD}/data/trimmedReads”
output_dir="${PWD}/Seq_data/data/trimmedReads/rsem_results”
annotation_dir=/scratch/alpine/kfotso@xsede.org/Seq/annotation/hg38
rsem_ref_dir="$annotation_dir/rsem_ref”
star_genome_dir="$annotation_dir/star_genome”
log_dir="${PWD}/AnkleOA_RNA_Seq/blood_data/trimmedReads/logs"
```

Export directories

Let’s submit a container application slurm script

- You mind need to bind some key directories or filesystems that you will export inside your container when running it.

```
apptainer exec -H $CONTAIN_DIR --bind=$input_dir,$output_dir \
$CONTAIN_DIR/RNA_seq_updated_STAR.sif STAR –runMode genomeGenerate \
--quantMode TranscriptomeSAM \
--genomeDir "$star_genome_dir" \
--genomeFastaFiles "rsem_ref/GRCh38.primary_assembly.genome.fa" \
--sjdbGTFfile "gencode.v47.annotation.gtf" \
--sjdbOverhang 100 \
--runThreadN $SLURM_NTASKS
```

exec is a command that will directly run the container Image.

Let’s submit a container application slurm script

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```
apptainer exec -H $CONTAIN_DIR --bind=$input_dir,$output_dir \
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--sjdbGTFfile "gencode.v47.annotation.gtf" \
--sjdbOverhang 100 \
--runThreadN $SLURM_NTASKS
```

exec is a command that will directly run the container image.

This command works with singularity as well.

Let’s submit a container application slurm script

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```
apptainer exec -H $CONTAIN_DIR --bind=$input_dir,$output_dir \
$CONTAIN_DIR/RNA_seq_updated_STAR.sif STAR –runMode genomeGenerate \
--quantMode TranscriptomeSAM \
--genomeDir "$star_genome_dir" \
--genomeFastaFiles "rsem_ref/GRCh38.primary_assembly.genome.fa" \
--sjdbGTFfile "gencode.v47.annotation.gtf" \
--sjdbOverhang 100 \
--runThreadN $SLURM_NTASKS
```

Specify a home directory as the $CONTAIN_DIR variable

Let’s submit a container application slurm script

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```
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--sjdbGTFfile "gencode.v47.annotation.gtf" \
--sjdbOverhang 100 \
--runThreadN $SLURM_NTASKS
```

We can bind additional directories and filesystems with --bind

Let’s submit a container application slurm script

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```
apptainer exec -H $CONTAIN_DIR --bind=$input_dir,$output_dir \
$CONTAIN_DIR/RNA_seq_updated_STAR.sif STAR –runMode genomeGenerate \
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--genomeDir "$star_genome_dir" \
--genomeFastaFiles "rsem_ref/GRCh38.primary_assembly.genome.fa" \
--sjdbGTFfile "gencode.v47.annotation.gtf" \
--sjdbOverhang 100 \
--runThreadN $SLURM_NTASKS
```

Path to our STAR sif image where we call STAR.

Let’s submit a container application slurm script

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```
apptainer exec -H $CONTAIN_DIR --bind=$input_dir,$output_dir \
$CONTAIN_DIR/RNA_seq_updated_STAR.sif STAR –runMode genomeGenerate \
--quantMode TranscriptomeSAM \
--genomeDir "$star_genome_dir" \
--genomeFastaFiles "rsem_ref/GRCh38.primary_assembly.genome.fa" \
--sjdbGTFfile "gencode.v47.annotation.gtf" \
--sjdbOverhang 100 \
--runThreadN $SLURM_NTASKS
```

Note that we can call our number of tasks with $SLURM_NTASKS.

For #SBATCH --cpus-per-task, you may use

$SLURM_CPUS_PER_TASK

How to run singularity on a gpu partition?

- Here, we take an example using a deepvariant container image on Alpine from here: https://github.com/google/deepvariant/blob/r1.6.1/docs/deepvariant-quick-start.md

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```
#!/bin/bash
#SBATCH --job-name=deepvariant_gpu
#SBATCH --nodes=1
#SBATCH --ntasks=16 # This is to select the amount of cores for the part of your code that will run on the CPU
#SBATCH --time=24:00:00  # This is to change the walltime
#SBATCH --partition=aa100 # Name of the NVIDIA gpu partition
#SBATCH --gres=gpu:1 # Requesting 1 GPU from the GPU node (There is a total of 3 gpus per node)
#SBATCH --constraint=gpu80
#SBATCH --output=deepvariant_gpu-%j.out
#SBATCH --error=deepvariant_gpu-%j.err
#SBATCH --qos=normal
```

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#SBATCH --ntasks=16 # This is to select the amount of cores for the part of your code that will run on the CPU
#SBATCH --time=24:00:00  # This is to change the walltime
#SBATCH --partition=aa100 # Name of the NVIDIA gpu partition
#SBATCH --gres=gpu:1 # Requesting 1 GPU from the GPU node (There is a total of 3 gpus per node)
#SBATCH --constraint=gpu80 # This will select only gpu nodes with 80G VRAM per gpu.
#SBATCH --output=deepvariant_gpu-%j.out
#SBATCH --error=deepvariant_gpu-%j.err
#SBATCH --qos=normal
```

How to run singularity on a gpu partition?

- Here, we take an example using a deepvariant container image on Alpine from here: https://github.com/google/deepvariant/blob/r1.6.1/docs/deepvariant-quick-start.md
- In this case, there are some system environment variable and paths that we needed to export. We call it myenvs:

```
LD_LIBRARY_PATH=/usr/local/lib/python3.8/dist-packages/nvidia/cublas/lib:/usr/local/nvidia/lib:/usr/local/nvidia/lib64:/.singularity.d/libs
TMPDIR=/gpfs/alpine1/scratch/kfotso@xsede.org/mytmp
```

How to run singularity on a gpu partition?

- Here, we take an example using a deepvariant container image on Alpine from here: https://github.com/google/deepvariant/blob/r1.6.1/docs/deepvariant-quick-start.md
- Then , we can run our container, assuming that we have exported all the tmp variables and defined all the directory variables to bind as well.

```
apptainer exec -H $CONTAIN_DIR --
bind=$CONTAIN_DIR,$ALPINE_SCRATCH,$RESULT_DIR,$LONG_READ_DIR,$TMPDIR

--nv

--env-file myenvs \ deepvariant-gpu-1_6_1_v2.sif /opt/deepvariant/bin/run_deepvariant \

--model_type=MODEL --ref=$REF --reads=$READS \

--output_vcf=$RESULT_DIR/mydata.vcf.gz \

--intermediate_results_dir $ALPINE_SCRATCH/intermediate_results_dir

--sample_name=SAMPLE --num_shards=$SLURM_NTASKS
```

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apptainer exec -H $CONTAIN_DIR --
bind=$CONTAIN_DIR,$ALPINE_SCRATCH,$RESULT_DIR,$LONG_READ_DIR,$TMPDIR

--nv

--env-file myenvs \

deepvariant-gpu-1_6_1_v2.sif /opt/deepvariant/bin/run_deepvariant \

--model_type=MODEL--ref=$REF --reads=$READS \

--output_vcf=$RESULT_DIR/mydata.vcf.gz \

--intermediate_results_dir $ALPINE_SCRATCH/intermediate_results_dir

--sample_name=SAMPLE --num_shards=$SLURM_NTASKS
```

--env-file allows to call directly those additional system variable directories into the container image, when running it.

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- Then , we can run our container, assuming that we have exported all the tmp variables and defined all the directory variables to bind as well.

```
apptainer exec -H $CONTAIN_DIR --
bind=$CONTAIN_DIR,$ALPINE_SCRATCH,$RESULT_DIR,$LONG_READ_DIR,$TMPDIR
--nv
--env-file myenvs \
deepvariant-gpu-1_6_1_v2.sif /opt/deepvariant/bin/run_deepvariant \
--model_type=MODEL--ref=$REF --reads=$READS \
--output_vcf=$RESULT_DIR/mydata.vcf.gz \
--intermediate_results_dir $ALPINE_SCRATCH/intermediate_results_dir
--sample_name=SAMPLE--num_shards=$SLURM_NTASKS
```

--nv allows to mount nvidia cuda related libraries from your host env into your container env.

How to modify/edit a container image on Alpine?

- In this case, we modify a container image that runs on an AMD gpu on Alpine.

Use the commands below to access respectively an AMD gpu debug node and and AMD batch node.

sinteractive ***--partition=atesting_mi100*** *--qos=testing --time=01:00:00 --gres=gpu:1 --ntasks=4*

sinteractive ***--partition=ami100*** *--nodes=1 --ntasks=4 --gres=gpu:1 --time=00:10:00 –reservation=amc_workshop*

How to modify/edit a container image on Alpine?

- To build the container, we have to create an overlay. An overlay is a filesystem that is going to be mounted on top of the container and serve as a buffer to edit the container image.

- If you modify a .sif or .simg container image via an overlay, you will always need to call it from now on, as it retains all the edits.

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- In this case, we try to build and modify and AMD gpu container.

apptainer build dev-ubuntu-20.04_latest.sif docker://rocm/dev-ubuntu-20.04_latest

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```
apptainer build dev-ubuntu-20.04_latest.sif docker://rocm/dev-ubuntu-20.04_latest
```

```
apptainer overlay create --fakeroot --sparse --size 100000 sparse_simple_overlay.img
```

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```

```
apptainer overlay create --fakeroot --sparse --size 100000 sparse_simple_overlay.img
```

Sparse overlay only takes up space on disk as data is written over it.

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```

```
apptainer overlay create --fakeroot --sparse --size 100000 sparse_simple_overlay.img
```

100000 MiB size

How to modify/edit a container image on Alpine?

- To build the container, we have to create an overlay. An overlay is a filesystem that is going to be mounted on top of the container and serve as a buffer to edit the container image.

- If you modify a .sif or .simg container image via an overlay, you will always need to call it from now on, as it retains all the edits.

- In this case, we try to build and modify and AMD gpu container.

```
apptainer build dev-ubuntu-20.04_latest.sif docker://rocm/dev-ubuntu-20.04_latest
```

```
apptainer overlay create --fakeroot --sparse --size 100000 sparse_simple_overlay.img
```

- Allows user to build root without sudo priviledges and interact with the overlay

How to modify/edit a container image on Alpine?

```
echo "********************************* Copying the .sif and .img files  *************************"
cp /scratch/alpine/kfotso@xsede.org/test_container_docker/sparse_3_simple_overlay.img .
cp /scratch/alpine/kfotso@xsede.org/test_container_docker/build-dev-ubuntu-20.04_latest.sif .
export CONTAIN_DIR=${PWD}

echo "********************************* Running the built container *************************"
# --containall is very important as it allows to transfer video permission to the container
# Otherwise you will not see the AMD GPU
#--overlay allows to create a filesystem on top of the immutable .sif container
# so that you can modify it at will with the --fakeroot option
# To install packages and run pipeline inside the container we run:
apptainer shell -H $CONTAIN_DIR --bind=/dev/kfd,/dev/dri --fakeroot --rocm --containall --overlay sparse_3_simple_overlay.img build-dev-ubuntu-20.04_
```

--rocm is the equivalent of –nv for nvidia and allows to import system related AMD gpu libraries from the host into the container. call

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```

With shell, one can modify the container interactively and thus install packages, test software etc …

How to modify/edit a container image on Alpine?

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```

We export important filesystems necessary to run an AMD gpu inside a container.

How to modify/edit a container image on Alpine?

- Inside the container image, we copy a python script to /usr/bin to run it.

```
[kfotso@xsede.org@c3gpu-c2-u17 test_container_docker]$ apptainer shell -H $CONTAIN_DIR --bind=/dev/kfd,/dev/dri --fakeroot --rocm --containall --overlay spars
e_3_simple_overlay.img build-dev-ubuntu-20.04_latest.sif
]INFO:    User not listed in /etc/subuid, trying root-mapped namespace
INFO:    Using fakeroot command combined with root-mapped namespace
WARNING: Skipping /dev/kfd bind mount: already mounted
WARNING: Skipping /dev/dri bind mount: already mounted
INFO:    unknown argument ignored: lazytime
Apptainer> ]     ds
Apptainer>
Apptainer> cp tensors.py /usr/bin/
```

We are inside the apptainer shell.

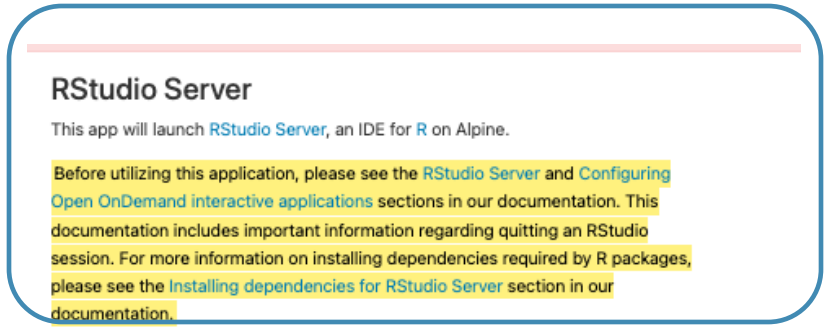
Rstudio on Alpine

What is Ondemand Rstudio?

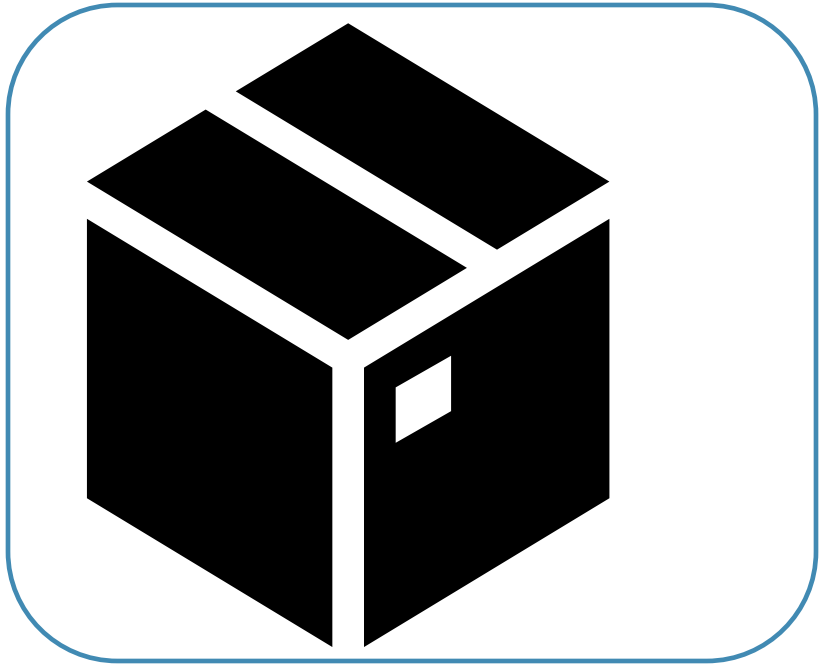
- It was built on top of an apptainer container image, thus, it runs on a different operating system than Alpine.

- A container is a tool that allows you to run different applications that were built on different operating systems on Alpine.

- The Rstudio .sif image is located at */curc/sw/containers/open_ondemand/rstudio-server-4.4.1.sif*



Rstudio



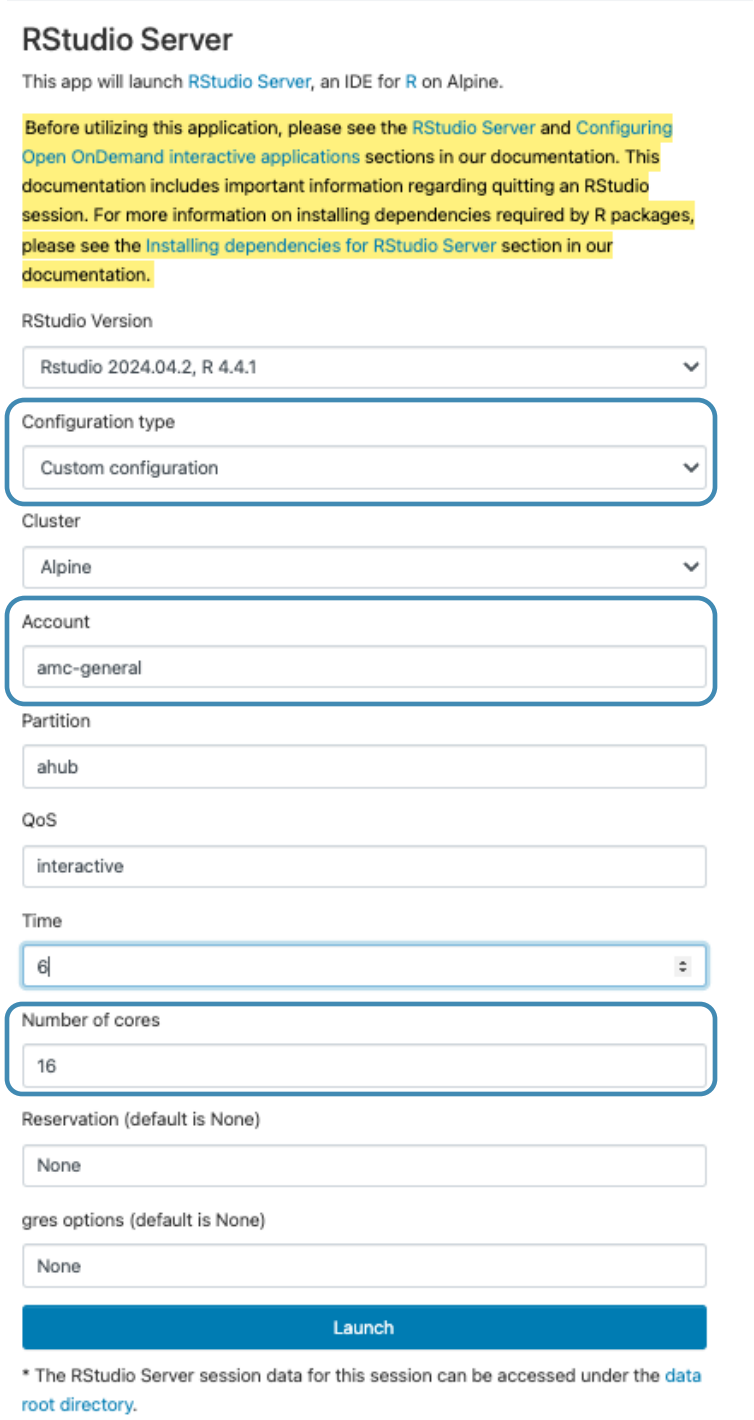
Container

Rstudio on Alpine

Use Rstudio on Alpine if:

- If you are used to Rstudio outside of Alpine
- You will need access to a GUI.
- If you think that most of your pipelines will not require more than 16 cores or 60GB of RAM.
- **Note: *** If you are new to Rstudio on Alpine, please refer to this guide: https://github.com/kf-cuanschutz/CU-Anschutz-HPC-documentation/tree/main/Rstudio_related_scripts

* If you wish to run your Rstudio contained environment as a slurm batch script, please refer to this guide: https://github.com/kf-cuanschutz/CU-Anschutz-HPC-documentation/blob/main/Rstudio_on_Slurm_.md



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Container orchestration

- An easy way to orchestrate if you are running a container image with multiple similar like files is to use job arrays.

Container orchestration

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#!/bin/bash

#SBATCH --nodes=1

#SBATCH --ntasks=10 # Number of CPU cores. As you request more CPU cores, you are also getting more CPU memory. ***You have about 3.8G per core***

#SBATCH --time=03:00:00 # Walltime

#SBATCH --partition=aa100 # This is the name of the NVIDIA GPU partition. Made of nodes containing 3x A100 gpus.

#SBATCH --gres=gpu:1 # Here we are requesting 1 gpu
#SBATCH --job-name=cellbender_gpu # Name of the job that will be submitted.

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#SBATCH --array=1-72

We add *add into the slurm header which correspond to the number of samples.*

Container orchestration

- An easy way to orchestrate if you are running a container image with multiple similar like files is to use job arrays.

```
export IndexID=$SLURM_ARRAY_TASK_ID
```

Then, we fetch the array task index corresponding to the slurm array subjobID:

Container orchestration

- An easy way to orchestrate if you are running a container image with multiple similar like files is to use job arrays.

```
export IndexID=$SLURM_ARRAY_TASK_ID
export SAMPLE="RESULT_${IndexID}"
mkdir $SAMPLE
export Data_dir=/pl/active/foolab/shared/$SAMPLE
```

We assign it to a variable called SAMPLE

```
apptainer exec -H $CONTAIN_DIR --
bind=$Data_dir,$ALPINE_SCRATCH,$SAMPLE
--nv \
cellbender_gpu.sif cellbender remove-background \
--cuda  --fpr 0.1  --input $Data_dir/raw_feature_bc_matrix.h5 \
--output $SAMPLE/output.h5
```

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export SAMPLE="RESULT_${IndexID}"

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export Data_dir=/pl/active/foolab/shared/$SAMPLE
```

Exporting data where the sample ID is located

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apptainer exec -H $CONTAIN_DIR --
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--cuda  --fpr 0.1  --input $Data_dir/raw_feature_bc_matrix.h5 \
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```

Exporting the array ID properly into the container image


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THANK YOU