Bioinformatics Containerization Tutorial
Session 3: DockerHub and Apptainer (KUACC)

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1 Overview

In this session you will:

- Tag, log in, and push your image to Docker Hub.
- Convert the Docker image into an Apptainer `.sif` file.
- Transfer the `.sif` file to KUACC.
- Bind KUACC directories into the container.
- Run ANGSD/PCAngsd inside Apptainer interactively.

2 Tag, log in, and push to Docker Hub

We assume you have a local image:

```
docker images
```

Example:

```
REPOSITORY        TAG       IMAGE ID       CREATED        SIZE
isophya-course    0.1       8c0a92d3f0a2   12 hours ago   6.3GB
```

2.1 Log in to Docker Hub

```
docker login -u iksaglam
```

When prompted, use a Personal Access Token (PAT) with read/write scope.

Verify:

```
docker info | grep Username
```

2.2 Tag the image

```
docker tag isophya-course:0.1 iksaglam/isophya-course:0.1
```

2.3 Push the image

```
docker push iksaglam/isophya-course:0.1
```

Anyone can later run:

```
docker pull iksaglam/isophya-course:0.1
```

3   Build the Apptainer image locally

On your laptop (with Apptainer installed):

```
apptainer build isophya-course_0.1.sif \
  docker://iksaglam/isophya-course:0.1
```

This produces:

```
ls -lh isophya-course_0.1.sif
```

4   Transfer the `.sif` file to KUACC

```
scp isophya-course_0.1.sif \
  iksaglam@login.kuacc.ku.edu.tr:~/oulu/
```

On KUACC:

```
ssh iksaglam@login.kuacc.ku.edu.tr
cd ~/oulu
ls -lh isophya-course_0.1.sif
```

5   Create runtime directories on KUACC

Inside `~/oulu`:

```
mkdir -p ~/oulu/data
mkdir -p ~/oulu/results
mkdir -p ~/oulu/scripts
```

Place into:

- `~/oulu/data`: .bamlist, .sites, .chr, .info, .clst, etc.

- `~/oulu/results`: empty directory for outputs.

- `~/oulu/scripts`: copies of `01_call_genotypes.sh`, `02_pcangsd_pipeline.sh`, `pcadapt.R`, `plotPCA.R`, `plotAdmix.R`.

Large data remain where they already live:

```
/userfiles/utopalan22/isophya/new_bams
/userfiles/utopalan22/isophya/references
```

6   Binding layout inside the container

We choose:

Host path	Container path	Use
~/oulu/data	/data	metadata, lists, filters
/userfiles/.../new_bams	/data/bams	BAMs (large)
/userfiles/.../references	/data/ref	reference genome
~/oulu/results	/results	outputs
~/oulu/scripts	/workspace/scripts	scripts

This matches the defaults in your scripts, for example:

```
REF="${REF:-/data/ref/isophya_contigs_CAYMY.fasta}"
```

7 Inspect and run Apptainer on KUACC

7.1 Inspect the image

```
cd ~/oulu
module load apptainer/1.4.1

apptainer inspect isophya-course_0.1.sif
```

7.2 Test bindings interactively

```
apptainer exec \
  --bind ~/oulu/data:/data:ro \
  --bind /userfiles/utopalan22/isophya/new_bams:/data/bams:ro \
  --bind /userfiles/utopalan22/isophya/references:/data/ref:ro \
  --bind ~/oulu/results:/results \
  --bind ~/oulu/scripts:/workspace/scripts:ro \
  isophya-course_0.1.sif \
  bash -lc 'ls /data; ls /data/bams | head; ls /data/ref; ls /workspace/scripts'
```

If this lists the expected files, your bindings are correct.

7.3 Interactive shell

```
apptainer shell \
  --bind ~/oulu/data:/data:ro \
  --bind /userfiles/utopalan22/isophya/new_bams:/data/bams:ro \
  --bind /userfiles/utopalan22/isophya/references:/data/ref:ro \
  --bind ~/oulu/results:/results \
  --bind ~/oulu/scripts:/workspace/scripts:ro \
  --pwd /workspace \
  isophya-course_0.1.sif
```

Inside:

```
angsd -h
python -m pcangsd -h
ls /data
```

```
ls /results
```

8 Run full pipelines interactively

8.1 ANGSD genotype calling

```
cd ~/oulu

apptainer exec \
  --bind ~/oulu/data:/data:ro \
  --bind /userfiles/utopalan22/isophya/new_bams:/data/bams:ro \
  --bind /userfiles/utopalan22/isophya/references:/data/ref:ro \
  --bind ~/oulu/results:/results \
  --bind ~/oulu/scripts:/workspace/scripts:ro \
  --pwd /workspace \
  isophya-course_0.1.sif \
  bash -lc './scripts/01_call_genotypes.sh'
```

8.2 PCAngsd + selection pipeline

```
cd ~/oulu

apptainer exec \
  --bind ~/oulu/data:/data:ro \
  --bind /userfiles/utopalan22/isophya/new_bams:/data/bams:ro \
  --bind /userfiles/utopalan22/isophya/references:/data/ref:ro \
  --bind ~/oulu/results:/results \
  --bind ~/oulu/scripts:/workspace/scripts:ro \
  --pwd /workspace \
  isophya-course_0.1.sif \
  bash -lc './scripts/02_pcangsd_pipeline.sh'
```

9 Summary

After Session 3 you can:

- Publish your image on Docker Hub.

- Build a portable Apptainer .sif file.

- Bind KUACC directories into the container.

- Run your ANGSD and PCAngsd workflows interactively on the cluster.