Analysis Pipeline on the Cloud

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Docker and AWS Batch

Presentation

- Overview
  - Docker
  - AWS Batch Service
- Importance of Docker
- Docker Images and the Analysis Pipeline
  - Summary of the Docker Images
  - Analysis Pipeline using AWS Batch Service
- Examples
  - Using Docker
  - Analysis Pipeline using AWS Batch Service

Docker Overview

- Platform for developing, deploying and running applications or systems
- A *Docker image* is:
  - built containing all software necessary to run the application
    - Usually built from a base image (e.g., *ubuntu*)
    - Includes all additional software to support an application or system (e.g., *gnu c/c++, python*)
    - Typically composed of multiple layers (e.g., *ubuntu layer, development tools layer, R layer*)
  - a read-only template with instructions for creating a *Docker container*

Docker Overview (cont)

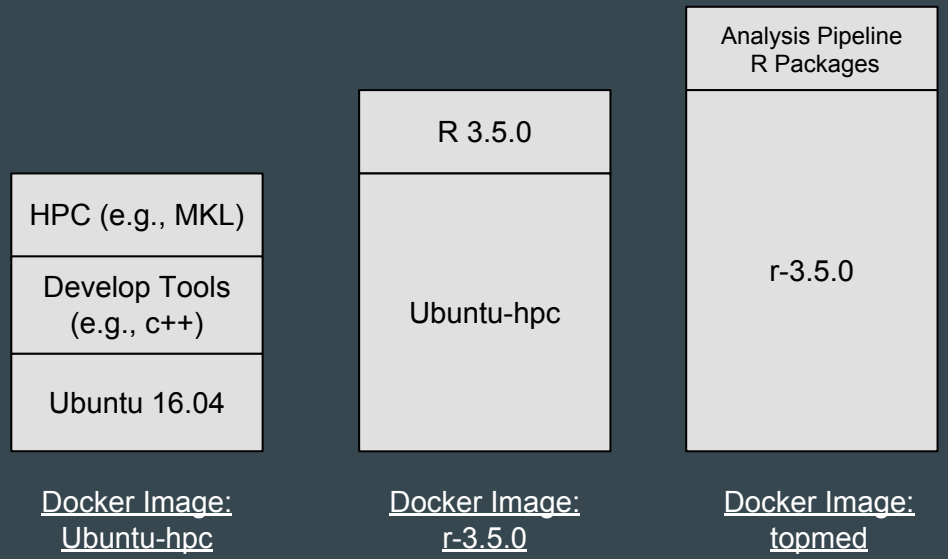
- A *Docker container* is:
  - a runnable instance of an image on a local or host computer (e.g., *Windows 10, macOS, Ubuntu*)
  - what the image becomes in memory when executed
  - runs natively on Linux
  - runs a Virtual Machine on *macOS* and *Windows* with access to host resources via a hypervisor
  - the container is considered *stateless* - when the container stops all changes to code and data are discarded (except for data on local host that is mapped to the container)

Docker Overview (cont)

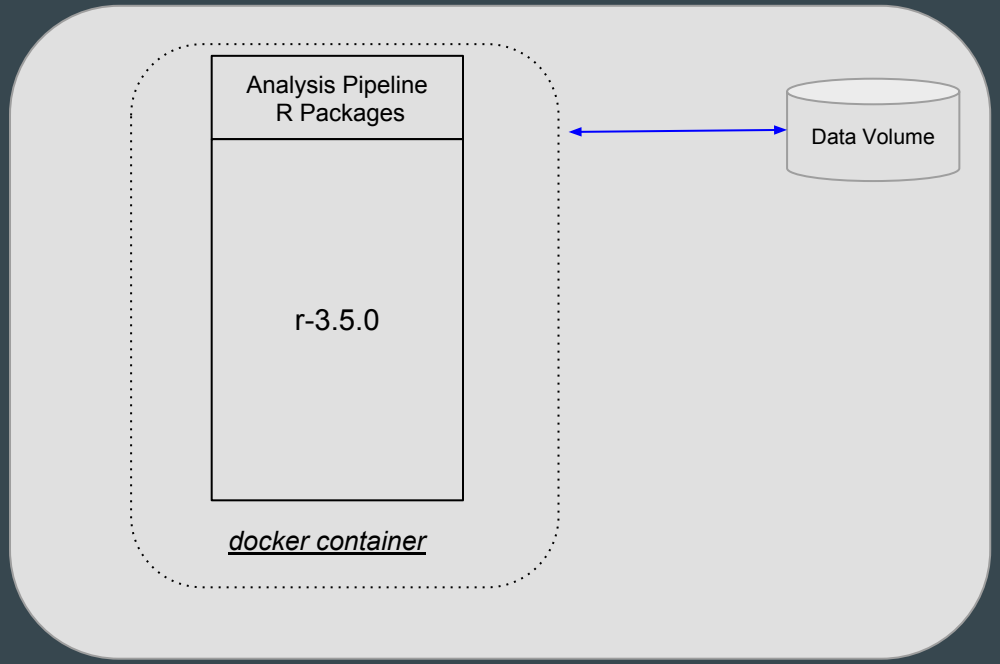
- What about accessing data on local host?
  - Data is typically not included in the *Docker image*
  - Data accessible on the local host can be mapped[1] (or *bind mounted*) to the *Docker container*
  - Any changes to data that is mapped to the local host is persisted when the *Docker container* stops

1. On *macOS*, file sharing is specified in the *Docker Preferences*

Docker Overview (Docker Images)

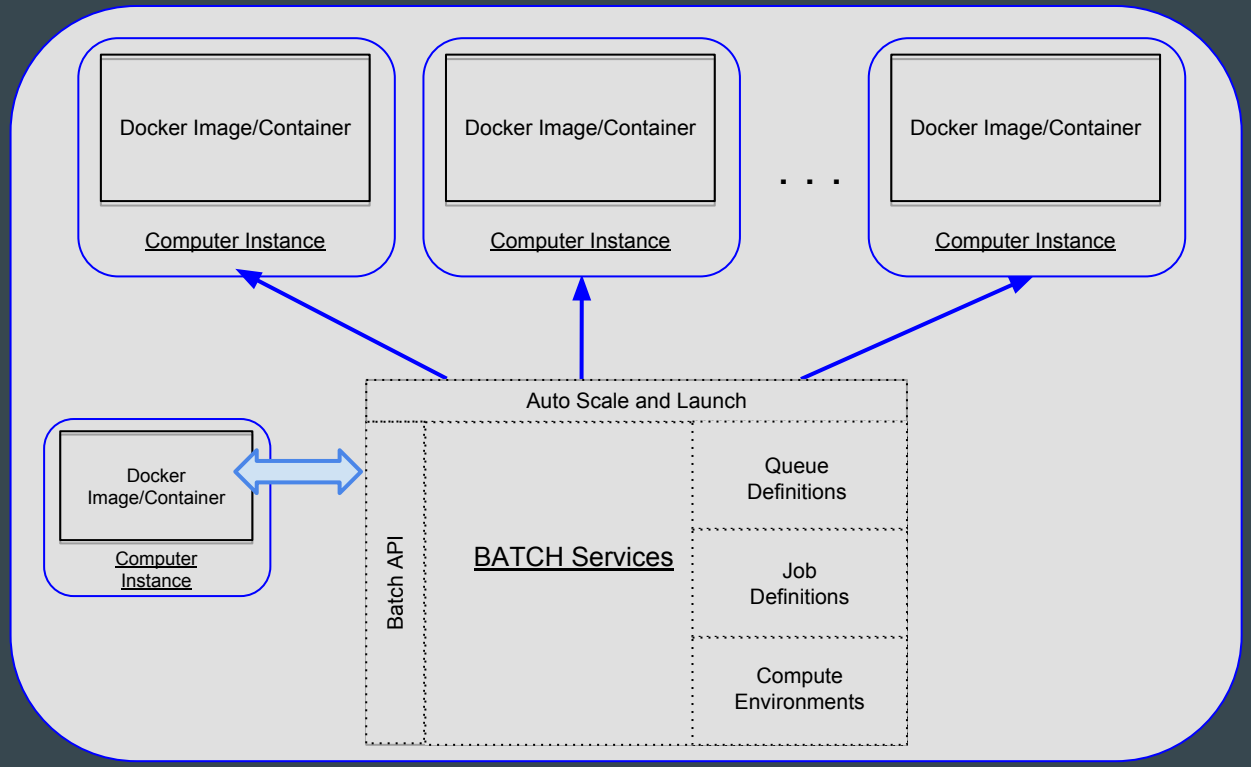


Docker Overview (Docker Container)



Linux, macOS or Windows
Computer

Overview AWS Batch Service



AWS Cloud

Importance of Docker (General)

- Develop a docker image with a completely configured system for running applications
- Deploy and run the same docker image on multiple platforms (e.g., *ubuntu, macOS, Windows)*
- Facilitates integrating applications in different environments (e.g., *AWS, Azure, Google Cloud, Seven Bridges*)
- Significantly reduces administrative cost in configuring computer systems to support the often numerous and diverse software required by applications

Importance of Docker (Analysis Pipeline)

- Easily deploy the base environment of software, libraries, and R packages associated with the analysis pipeline:
  - R
  - R packages
  - Math Kernel Library
  - Development environment (e.g., *c++*, *python*)
- Integrate with AWS Batch Services and its high-performance, parallel computing environment
- Integrate with *Seven Bridges Genomics*
- Potential to integrate in other high-performance, parallel computing environments

Docker Images and the Analysis Pipeline

- Summary of the *Docker Images*
  - uwgac/r-3.5.0-mkl
  - uwgac/topmed-master
  - uwgac/topmed-rstudio
- Analysis Pipeline using AWS Batch Service
  - Provide high performance data access
  - Integrate analysis pipeline with AWS batch service
  - Run the *Docker image* interactively

Analysis Pipeline using AWS Batch Service

- Provide high performance data access
  - Sharing data between computer instances via NFS
  - Mounting shared data to computer instances
  - Mapping shared data on computer instances to *Docker containers*

Analysis Pipeline using AWS Batch Service (cont)

- Integrate analysis pipeline with AWS batch service
  - Define jobs, queues, and compute environments in AWS batch service
  - Provide a *Docker image* to AWS batch service (job definition)
  - Within analysis pipeline (*AWS_Batch* class), utilize python API to submit jobs

Analysis Pipeline using AWS Batch Service (cont)

- Run the *Docker image* interactively
  - Copy AWS security credentials
  - Map shared data
  - Execute analysis pipeline commands (e.g., *assoc.py*)
  - Submit jobs to AWS Batch Service via python API

Examples - Using Docker

- Reference:
  https://uw-gac.github.io/topmed_workshop_2018/using-docker.html
- Example 1 - Running RStudio server

```
mkdir ~/workshop_2018
cd ~/workshop_2018
git clone https://github.com/uw-gac/docker_helpers
alias rs_docker='~/workshop_2018/docker_helpers/Rstudio_docker.py'
rs_docker

# connect via browser http://localhost:8787
```

Examples - Analysis Pipeline Using AWS Batch Services

- Reference:
  https://uw-gac.github.io/topmed_workshop_2018/analysis-pipeline.html#running-on-aws-batch
- Example

```
# connect to aws instance running docker
ssh -i ~/.ssh/xxx.pem kuraisa@52.27.98.54
# get docker helpers (done previously)
#git clone https://github.com/uw-gac/docker_helpers
alias pipeline='~/docker_helpers/analysis_pipeline.py'
# change working directory to shared data work folder
cd /projects/topmed/analysts/kuraisa/workshop/burden
pipeline --help
#
# run interactively docker image/container uwgac/topmed-master
# (similar to connecting to head node of a linux cluster)
#
pipeline
```

Examples - Analysis Pipeline Using AWS Batch Services (cont)

- Example (cont)

```
# now within the docker container (head node) - get info about job
# without submitting
/usr/local/analysis_pipeline/assoc.py \
 single testdata/assoc_window_burden.config \
  --cluster_type AWS_Batch \
  --cluster_file custom_batch.json --print  > single_burden_print.log
2>&1

more single_burden_print.log

# submit the job
/usr/local/analysis_pipeline/assoc.py \
 single testdata/assoc_window_burden.config \
  --cluster_type AWS_Batch \
  --cluster_file custom_batch.json  > single_burden.log  2>&1
```

Examples - Analysis Pipeline Using AWS Batch Services (cont)

- Example (cont)

```
# after submitting jobs,
# monitor from aws console (AWS Batch dashboard)

# wait for instance to start 5-10 mins
# (using spot may affect time)

# after job is running, view dashboard on console and
# list files on the "head" node
ls
```

Summary

- Overview of Docker and AWS Batch
- Importance of Docker
- Examples using Docker
- Example executing analysis pipeline on AWS Batch
- Next Presentation: Analysis Pipeline on *Seven Bridges Genomics*

Questions

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