

**MAKE YOUR LIFE
(AND ANALYSIS)
EASIER WITH
CONTAINERS**

AUDIENCE

- Are you a biologist?
- Have you heard of Docker?
- Not sure where to start?

YOU'VE COME TO THE RIGHT PLACE!

ME

- Software Engineer
- Build software infrastructure for researchers
- Help researchers to use computational tools
- Was a 'container skeptic'

CYVERSE

Helps researchers:

1. Learn about, and
2. Productively use

New tech like containers

ANALYSIS IS GETTING COMPLEX

- Multiple software packages (R, Python, etc.)
- With specific versions
- Have to work together
- On different platforms

THE PAIN

- Hard to install one-by-one
- Wasted effort and time
- Fragile, hard-to-reproduce analyses

HELP! MAKE IT STOP!

How we we make it easy to install & use things
consistently?

CONTAINERS! *

New packages & apps are increasingly available as containers (biocontainers, etc.)

CONCEPTS & TERMS

IMAGE

A self-contained, read-only 'snapshot' of your applications and packages, with all their dependencies

DOCKERFILE (OR SINGULARITY RECIPE)

Executable instructions (script) for:

- Creating an image
- Specifying the 'entry point' for the container

CONTAINER

- A 'running image'

DOCKER

- A server (daemon): Handles life cycle of images and containers
- A command-line client: To tell the server what to do

Download from: <https://www.docker.com/>

SINGULARITY

A way to run containers on HPC

WHAT ABOUT MY DATA?

Do not put your data in the image!

- Local data: 'Mount' it into a container when you start it
- Remote data: Pull into the container once it's running (e.g. CyVerse Data Store, S3, etc.)

COMPUTE RESOURCES

I need more!

Talk to us. There are a few options, and it depends on what you need.

SHARING CONTAINERS

Image registries

USING CONTAINERS

COMMAND LINE APP

TODO

1. Get image
2. Locate data
3. Run

WEB APP

TODO

1. Get image
2. Locate data
3. Run

CYVERSE SUPPORT FOR CONTAINERS

1. Command line (Atmosphere)
2. Interactive apps (VICE)
3. HPC (XSEDE & OSG)

SUMMARY

- Package your analysis pipeline in a single container
- Everyone in your lab can have a consistent environment

NEXT TIME

- How to build containers
- Running on different platforms
- Science applications

LINKS & REFERENCES

TODO

THANKS!

- Nirav Merchant
- Upendra Devisetty
- Tyson Swetnam
- Blake Joyce
- Eric Lyons
- Ariella Gladstein
- Tina Lee
- Mary Margaret Sprinkles

