



Linux Containers

"Tech Interest Group" Seminar
2023-12-07



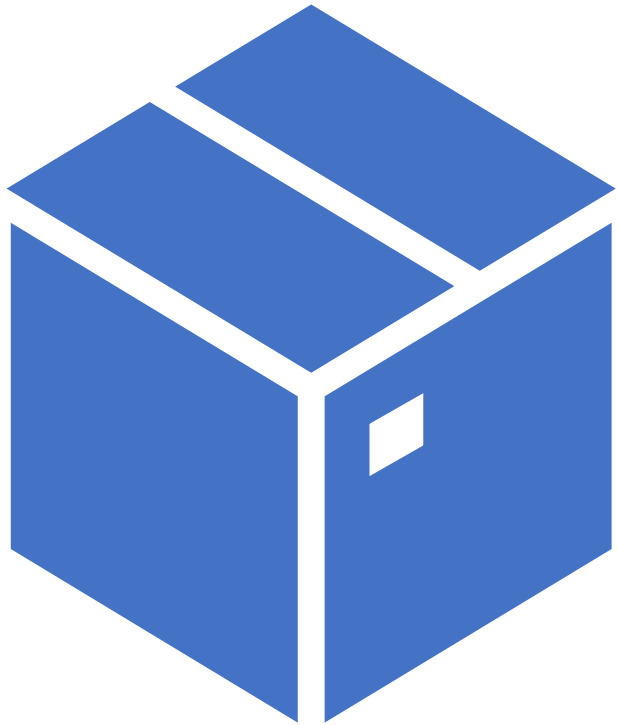
FNNDS
Fetal-Neonatal Neuroimaging
Developmental Science Center



- <https://bostonchildrens.zoom.us/j/95872814678?pwd=MW53RmVrRzNYRUh0czkvOFJjTHhldz09&from=addon>

Let's take a survey...

| Who uses... | Frequency |
|-------------------------|-----------|
| Docker | 1 |
| Apptainer (Singularity) | 3 |
| Podman | 0 |
| ChRIS | 3 |
| E2 | 3 |
| mghpcc | 0.5 |

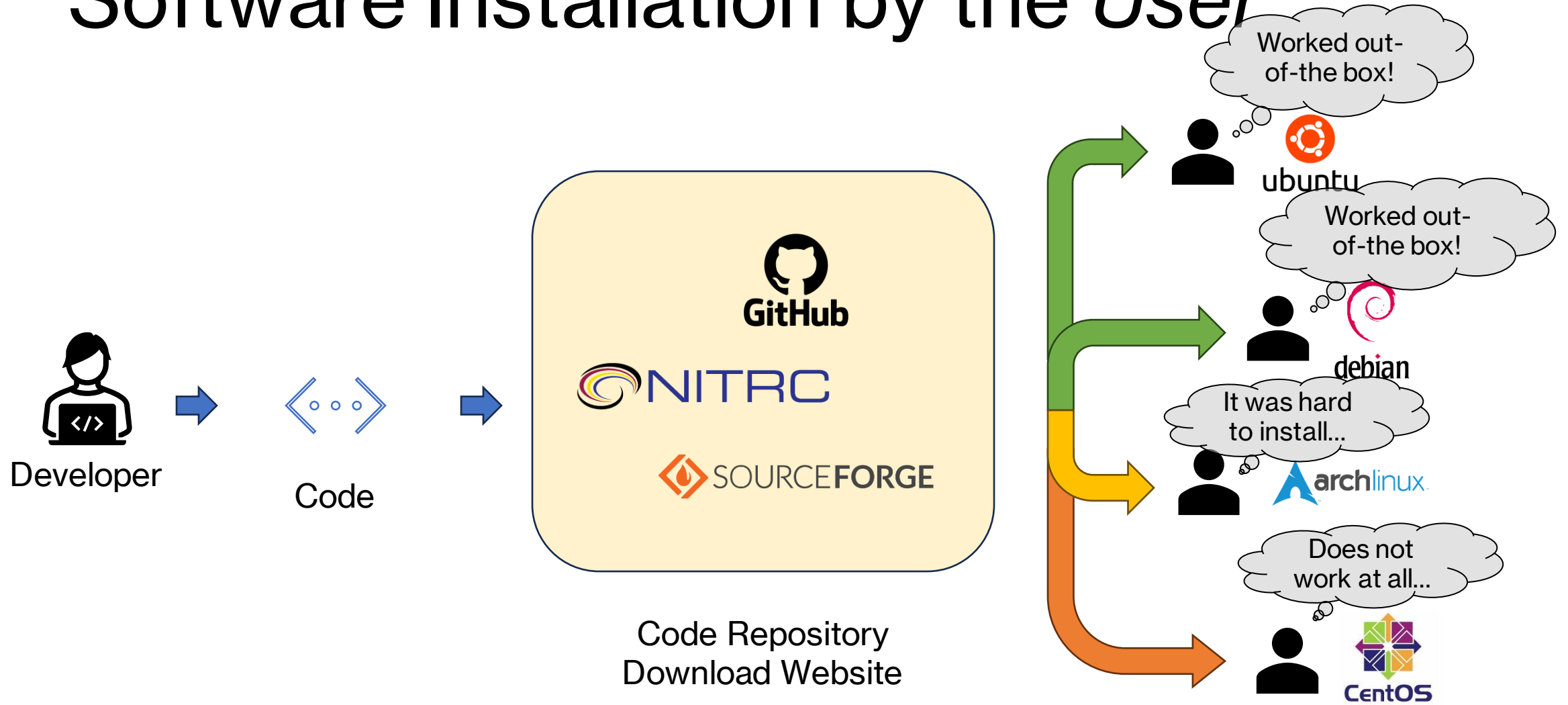


Why Containers
Portability

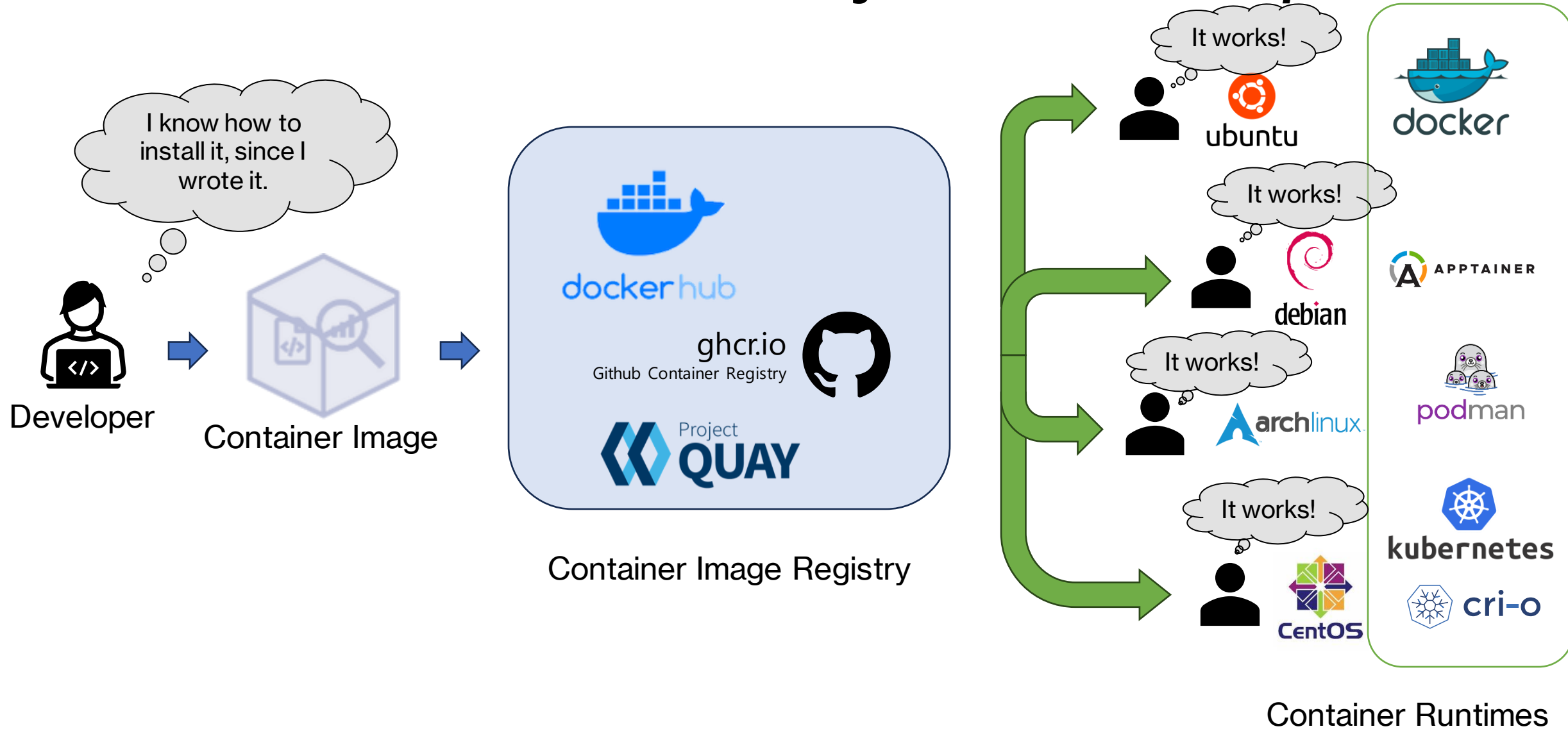
“It Works on My Machine.”

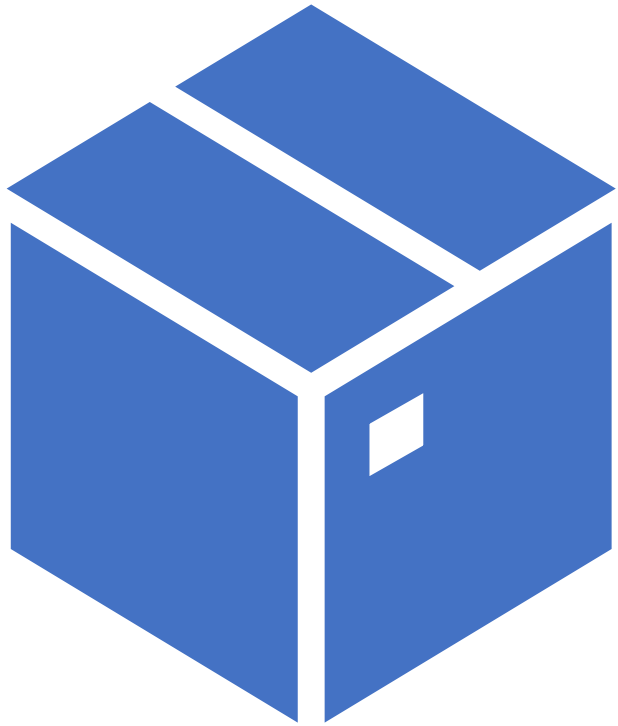
- Python:
 - `ModuleNotFoundError: No module named 'numpy'`
 - `AttributeError: 'MaskedArray' object has no attribute 'mini'`
- Compiled programs:
 - `error while loading shared libraries: libjbig.so.0: cannot open shared object file: No such file or directory`
 - `/lib/x86_64-linux-gnu/libc.so.6: version `GLIBC_2.28' not found`

Software Installation by the *User*



Software Installation by the *Developer*





Why Containers

Compatibility

Host

FreeSurfer v7.3.2

Depends on

Python v3.8.11

Tensorflow v1.6

Doesn't work with



Host

FreeSurfer v7.3.2

Python v3.8.11

Container #1

Tensorflow v1.15

Python v3.6.9

Container #2

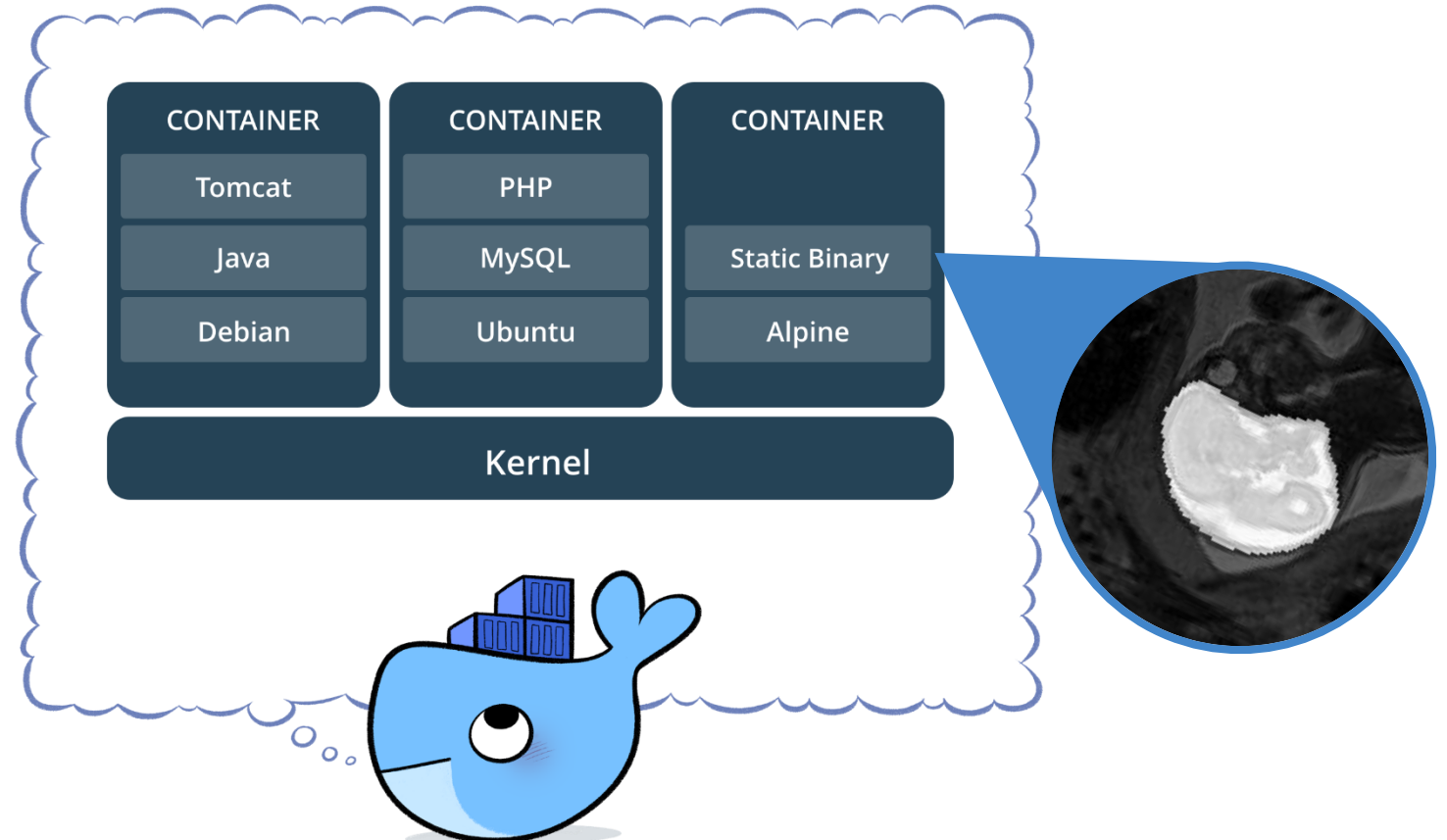
Tensorflow v2.12

Python v3.10.12

Container #3

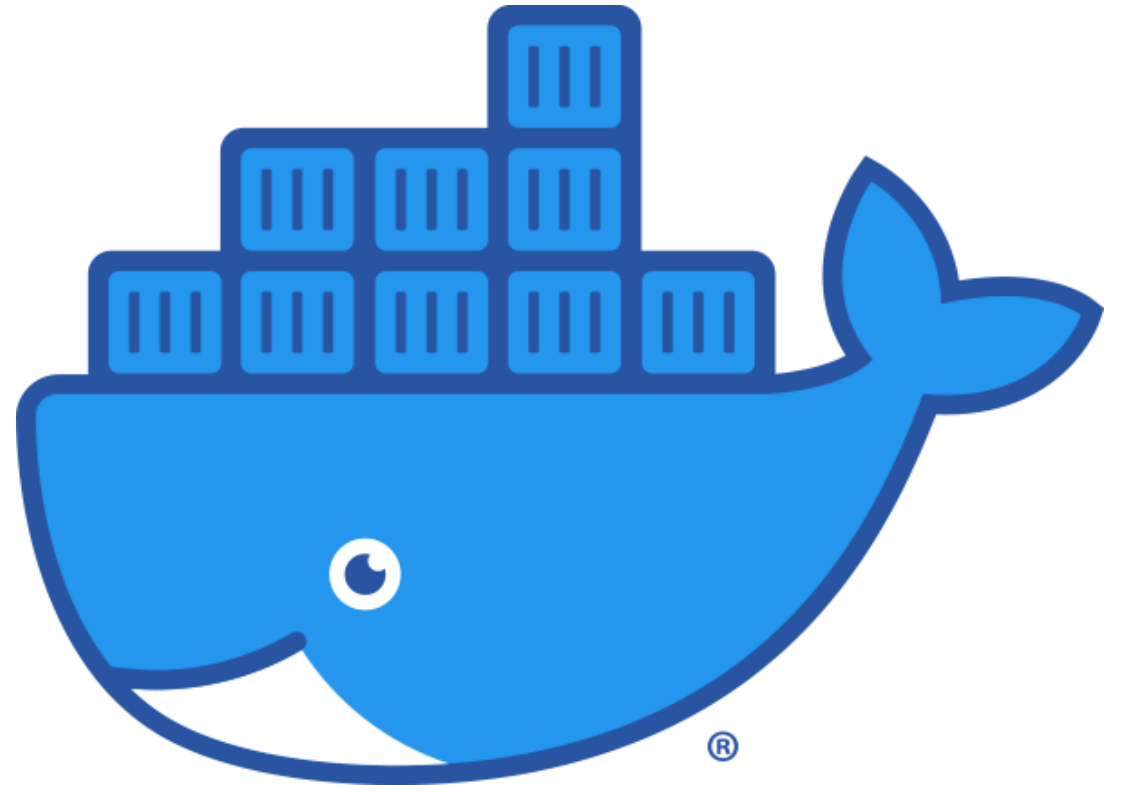
Why Containers?

- Portability
- Compatibility
- Reproducibility
- Security



What is... Docker?

- **Docker ≠ container**
- Docker is...
 - A company: Docker, Inc.
 - A “container runtime” (dockerd, docker.service)
 - A command you can run (docker)



How to use Docker

```
docker run freesurfer/freesurfer:7.3.2 recon-all
```

Where is my data?



How to use Docker (try 2)

```
docker run \  
  -v ~/subjects:/subjects \  
  -e SUBJECTS_DIR=/subjects \  
  freesurfer/freesurfer:7.3.2 recon-all
```

Why's everything
owned by root?



How to use Docker (try 3)

```
docker run \  
  -u $(id -u):$(id -g) \  
  -v ~/subjects:/subjects \  
  -e SUBJECTS_DIR=/subjects \  
  freesurfer/freesurfer:7.3.2 recon-all ...
```

Other stuff not
working...



How to use Docker (try ∞)

```
docker run \  
  --rm \  
  -i -t --net=host \  
  -v /etc/timezone:/etc/timezone:ro \  
  -u $(id -u)$(id -g) \  
  -v /etc/passwd:/etc/passwd:ro \  
  -e HOME=/tmp \  
  -v ~/subjects:/subjects:rw \  
  -e SUBJECTS_DIR=/subjects \  
  freesurfer/freesurfer:7.3.2 recon-all ...
```

Container-related (next slide)

Isolation & security

Data

What you want to run



What does `--rm` do?

Images

- Can be copied, downloaded, or uploaded
- Immutable
- To run an image, you create a container of it
- Images are *built* from containers

Containers

- Exists only on your computer
- Mutable
- Can be started/running or stopped
- Containers are *created* from images

More than you would care to know...



Introducing Apptainer (Singularity)

```
docker run \  
  --rm \  
  -i -t --net=host \  
  -v /etc/timezone:/etc/timezone:ro \  
  -u $(id -u)$(id -g) \  
  -v /etc/passwd:/etc/passwd:ro \  
  -v ~/subjects:/subjects:rw \  
  -e HOME=/tmp \  
  -e SUBJECTS_DIR=/subjects \  
  freesurfer/freesurfer:7.3.2 recon-all  
...
```

```
apptainer exec \  
  docker://freesurfer/freesurfer:7.3.2 \  
  recon-all ...
```

Recommendation:
Use apptainer to run *containers*,
and docker to build *images*



Everywhere you can run containers

- Locally:

- `docker run --rm -it -u "$(id -u):$(id -g)" fnndsc/imagename command...`
- `apptainer exec docker://fnndsc/imagename command ...`

- On E2:

- `srun -A fnndsc -p bch-interactive --qos=interactive \`
 `-n 4 --mem=8GB --time=30:00 --pty /bin/bash`
 `apptainer exec docker://fnndsc/imagename command ...`

- Via *ChRIS*: <http://chris-next.tch.harvard.edu>

Add a New Node




This wizard allows you to add a node to a feed

Select a Plugin Version:

Select a compute environment:

Fill the form using a latest run of this plugin

Command Line Parameters:



Validate

Required Parameters (1 parameter)

--age *

Age in months of the FreeSurfer subject that is to be processed.

Cancel

Back

Add Node

Limitations of Containers

- Difficult to develop, debug
- Storage inefficient (especially Apptainer)
- Different GPUs work differently
- Graphical user interfaces are hard to run

FNNDSC “Tech Interest Group”

- Schedule
 - Intro to the FNNDSC
 - Intro to Containers
 - My First *ChRIS* plugin: Part 1

<https://chrisproject.org/docs/ChRISalis>