Docker for the modern scientist

What is Docker?

- a tool designed to make it easier to create, deploy, and run applications by using containers.
- Allows a developer to package up an application with all of the parts it needs, such as libraries and other dependencies, and ship it all out as one package.

Why should a scientist care?

- A sharable computing environment so that all members of your lab have access to the same tools.
- An easily replicable experiment that can be run from anywhere (like autoFR or adaptiveFR).
- An analysis pipeline with all of the necessary code to replicate figures and statistics from a published paper.
- An application that runs Jupyter server so that your class can access the data and software without installing anything locally.

How do I get started?

- Clone our github repo: git clone https://github.com/ ContextLab/CDL-tutorials.git
- Install Docker and Google Chrome
- Follow the tutorial in Dockerfile for a basic runthrough

What is a Dockerfile?

a set of instructions for building a docker image.

```
# simple example of a Dockerfile
FROM ubuntu: latest
MAINTAINER Contextual Dynamics Lab "contextualdynamics@gmail.com"
# install python and flask
RUN apt-get update
RUN apt-get install -y python python-pip wget
RUN pip install Flask
# add a script
ADD simple_server.py /home/simple_server.py
# set the working directory
WORKDIR /home
```

How do I build an image?

\$ docker build -t cdl.

docker command line tool

Tag (name)

this folder

How do I run it?

Assign a port name it

\$ docker run -it -p 99999:9999 —name CDL cdl

Run interactively

Reference to the image

How do I open it again?

attach your terminal to it



Start it

Summary

- Docker is a very useful tool to scientists because it allows us to share computing environments.
- Sharable computing env = easily replicable experiments, analysis pipelines, figures, etc.
- Please follow the tutorial outlined in the README to learn how to built a simple Docker image.