Containerization: Best Practices & Advanced Topics

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XSEDE
Extreme Science and Engineering Discovery Environment

Outline

- Lifecyle of a Container
  - Development vs. Production
  - Example Container
  - Reducing Container Sizes
- Deploying a Container
  - In the Cloud
  - On a Shared Resource
- Security
- Next Steps
  - Reproducible Containers
  - Container Orchestration

Lifecycle of a Container

Containers for Development vs. Production

1. **Production:** Containers as a software distribution method
   - Portability of a consistent environment for users
   - Easily distributed
   - Highly accessible
   - Pre-packaged software containers often require customization

Lifecycle of a Container

Containers for Development vs. Production

1. **Production:** Containers as a software distribution method
   - Portability of a consistent environment for users
   - Easily distributed
   - Highly accessible
   - Pre-packaged software containers often require customization
2. **Development:** Containers as a development environment
   - Builds a consistent environment early, including dependencies
   - Useful for teams of developers/researchers
   - Larger if including dev tools
   - Often requires cleanup for production

Lifecycle of a Container

Containers for Development vs. Production

Development

Production

Lifecycle of a Container

Containers for Development vs. Production

Development

- Contains dependencies, code, environment variables, etc.
- No real size limit: text editors, VNC, data visualization, etc.
- Code is changed and updated
- Runs can be varied and versatile to initiate

Production

Lifecycle of a Container

Containers for Development vs. Production

Development

- Contains dependencies, code, environment variables, etc.
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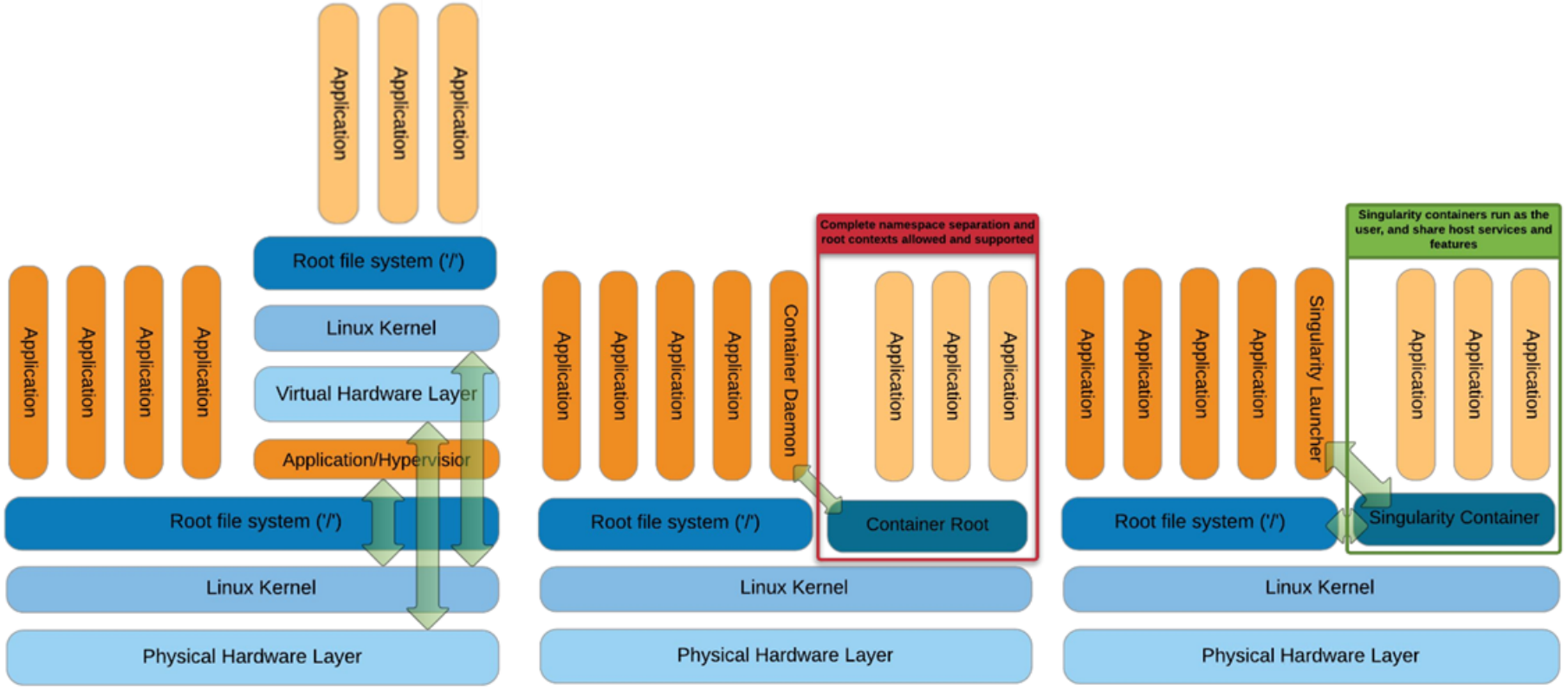
Production

- Contains dependencies, code, environment variables, etc.
- Should be as lightweight as possible: no need for nice aesthetic features
- Code is static
- Requires a run script or easy commands

Lifecycle of a Container

Data Management



Lifecycle of a Container

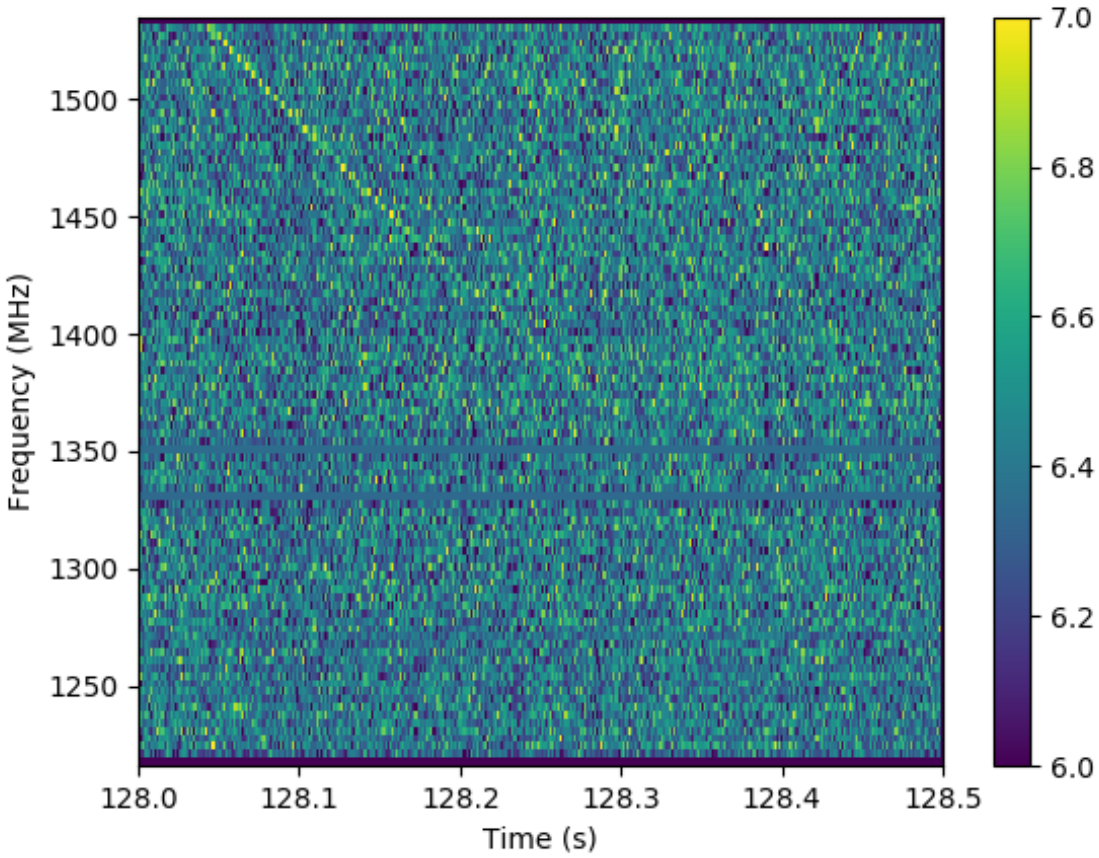
Data Management

- Manage data in Docker: https://docs.docker.com/storage/
  - Volumes https://docs.docker.com/storage/volumes/
  - Bind mounts https://docs.docker.com/storage/bind-mounts/
  - tmpfs mounts https://docs.docker.com/storage/tmpfs/

- Manage data in Singularity
  - Access to the root filesystem: https://sylabs.io/guides/3.5/user-guide/quick_start.html#working-with-files
  - Bind Paths and Mounts: https://sylabs.io/guides/3.5/user-guide/bind_paths_and_mounts.html
  - Persistent Overlays: https://sylabs.io/guides/3.5/user-guide/persistent_overlays.html

Lifecycle of a Container

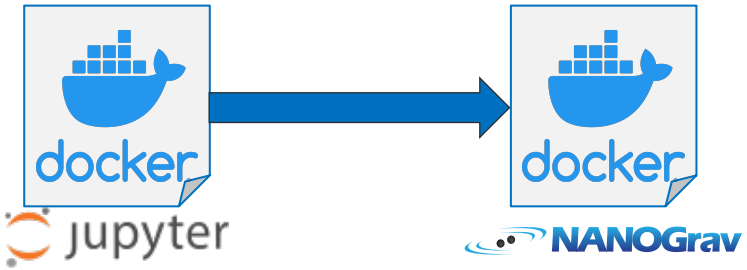
Example Container: Radio Astronomy



Lifecycle of a Container

Example Container: Radio Astronomy

- Started with a NANOGrav container: nanograv/nanopulsar
  - Based on jupyter/datascience-notebooks (includes Python, R, and more)
  - Wide variety of Radio Astronomy software and tools



Lifecycle of a Container

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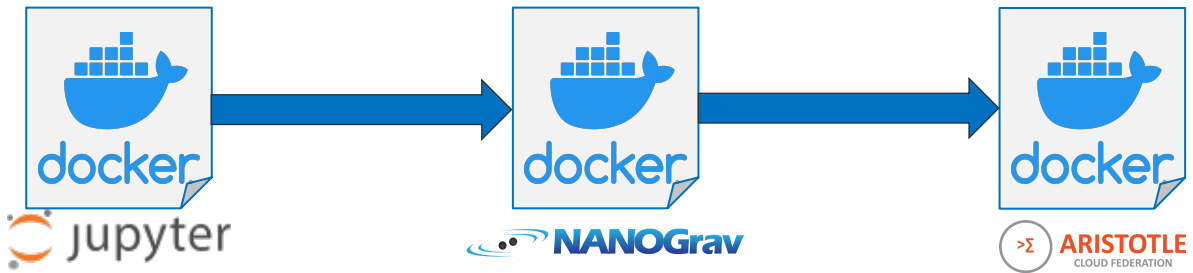
- After 1 year, needed to be updated: federatedcloud/nanopulsar
- Used for development with additions: federatedcloud/modulation_index
  - ~11GB for just dependencies



Lifecycle of a Container

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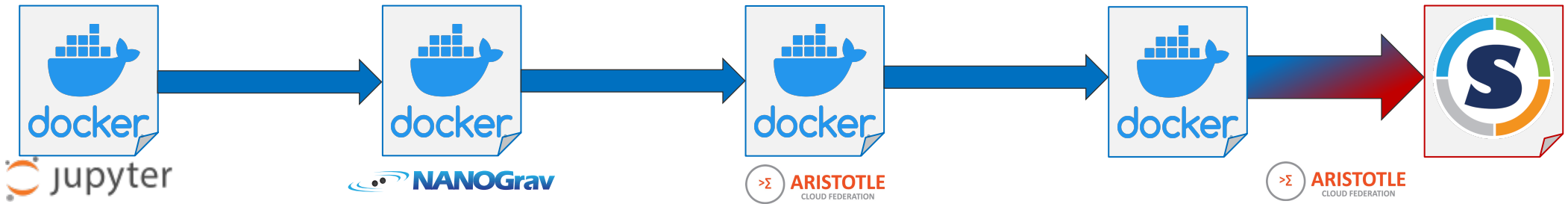
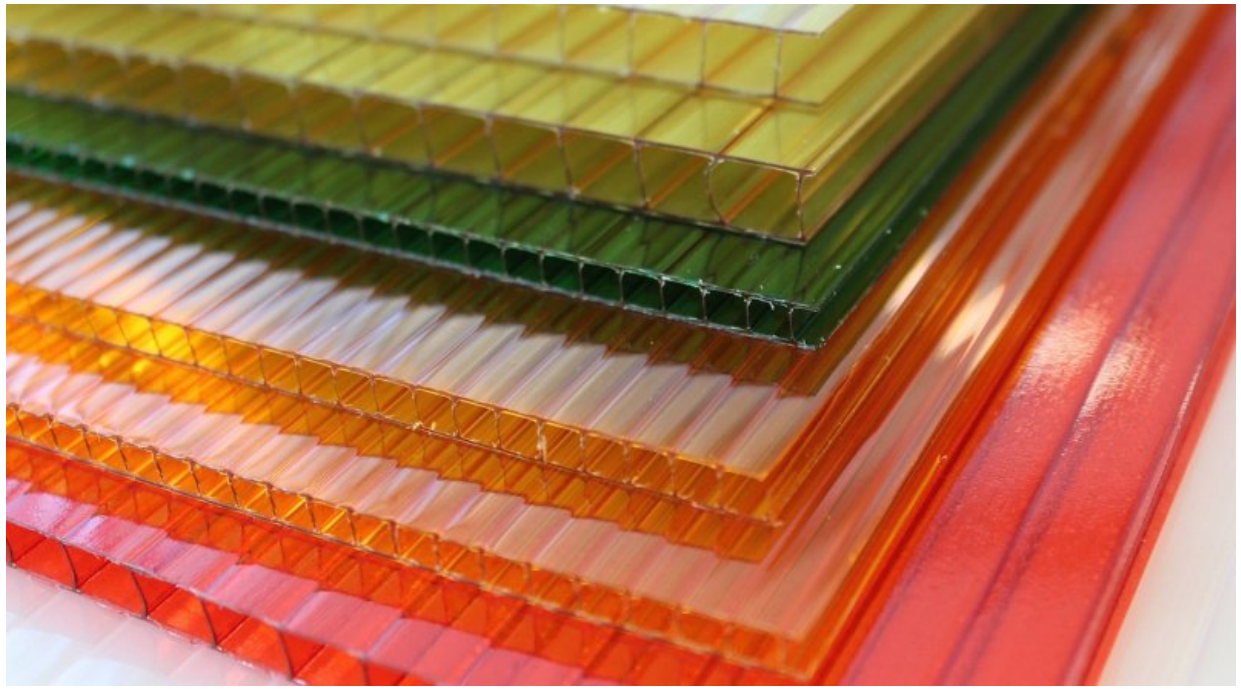
- After 1 year, needed to be updated: federatedcloud/nanopulsar
- Used for development with additions: federatedcloud/modulation_index
  - ~11GB for just dependencies
- Created a minimal container for production runs
  - ~3GB for just dependencies
  - Docker version: federatedcloud/docker-PRESTO
  - Singularity version: federatedcloud/singularity-PRESTO



Lifecycle of a Container

Reducing Container Sizes

- Docker Layers
  - Base image
    - CentOS 215MB
    - Debian 114MB
    - Ubuntu 73.9MB
    - Alpine 5.57MB
  - Certain commands add layers:
    RUN, ADD, COPY
  - 1 instruction = 1 layer
  - Other commands create temporary layers
  - Also see the Docker docs



Lifecycle of a Container

Reducing Container Sizes

- Combining multiple commands
  - Pip commands can use a requirements file

Our requirements.txt, for example:

```
alembic
fitsio==0.9.11
requests_oauthlib
marshmallow
ephem
scikit-sparse
corner
numexpr
astropy
runipy
…
```

Lifecycle of a Container

Reducing Container Sizes

- Combining multiple commands
  - Pip commands can use a requirements file
  - If using several RUN commands in a row, it's an opportunity to combine:

```
RUN wget -q https://bitbucket.org/psrsoft/tempo2/get/master.tar.gz && \
    tar zxf master.tar.gz && \
    cd psrsoft-tempo2-* && \
    ./bootstrap && \
    CPPFLAGS="-I/opt/pulsar/include" LDFLAGS="-L/opt/pulsar/lib" ./configure -- prefix=/opt/pulsar --with-calceph=/opt/pulsar && \
    make && make install && make plugins && make plugins-install && \
    mkdir -p /opt/pulsar/share/tempo2 && \
    cp -Rp T2runtime/* /opt/pulsar/share/tempo2/. && \
    cd .. && rm -rf psrsoft-tempo2-* master.tar.gz
```

Lifecycle of a Container

Reducing Container Sizes

- Combining multiple commands
  - Pip commands can use a requirements file
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- Use multi-stage builds
  - Leverages docker build cache

Lifecycle of a Container

Reducing Container Sizes

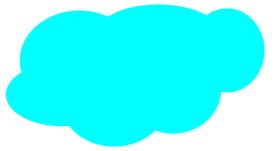
- Combining multiple commands
  - Pip commands can use a requirements file
  - If using several RUN commands in a row, it's an opportunity to combine
- Use multi-stage builds
  - Leverages docker build cache
- Don't install what you don't need
- Multiple decoupled containers (microservices)

Deploying a Container

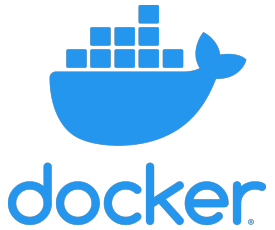
Best Practices for Uploading Containers

- Don’t upload
  - Private data – very important for research
  - Private or licensed software
- Do include
  - Software licenses
  - Documentation
  - Software and dependencies
  - Runscripts for production
- Use GitHub to connect your repo
  - DockerHub
  - SingularityHub

Deploying a Container
In the Cloud



- Will it work in the cloud?
  - Moving from HPC adds complexity
    - MPI
    - May require container orchestration
  - Data management
- Use Docker
  - Public cloud providers offer managed services
  - Container Orchestration options
  - Ease of use
- Security



Vaillancourt and Wineholt et al. 2020 PEARC20

Deploying a Container
On HPC Resources

- Simplifies getting started
  - No need to install to your home directory
  - No need to pester sysadmins to install your software
- Using Singularity on XSEDE
  - It's available and secure
  - Bind mounts for easy data access
  - Static container, no OverlayFS
- MPI **major version** in the container *must* match the host
  https://sylabs.io/guides/3.5/user-guide/mpi.html
- Job scripts and bind mounts may vary on different systems

Security

Root Access

- Use Singularity for sensitive systems
- Another option is Docker Rootless Mode
  - Docker Docs on Rootless Mode
  - DockerCon 2020 Talk on Rootless Mode
- Setup a user or users for shared Docker containers (same as shared system)

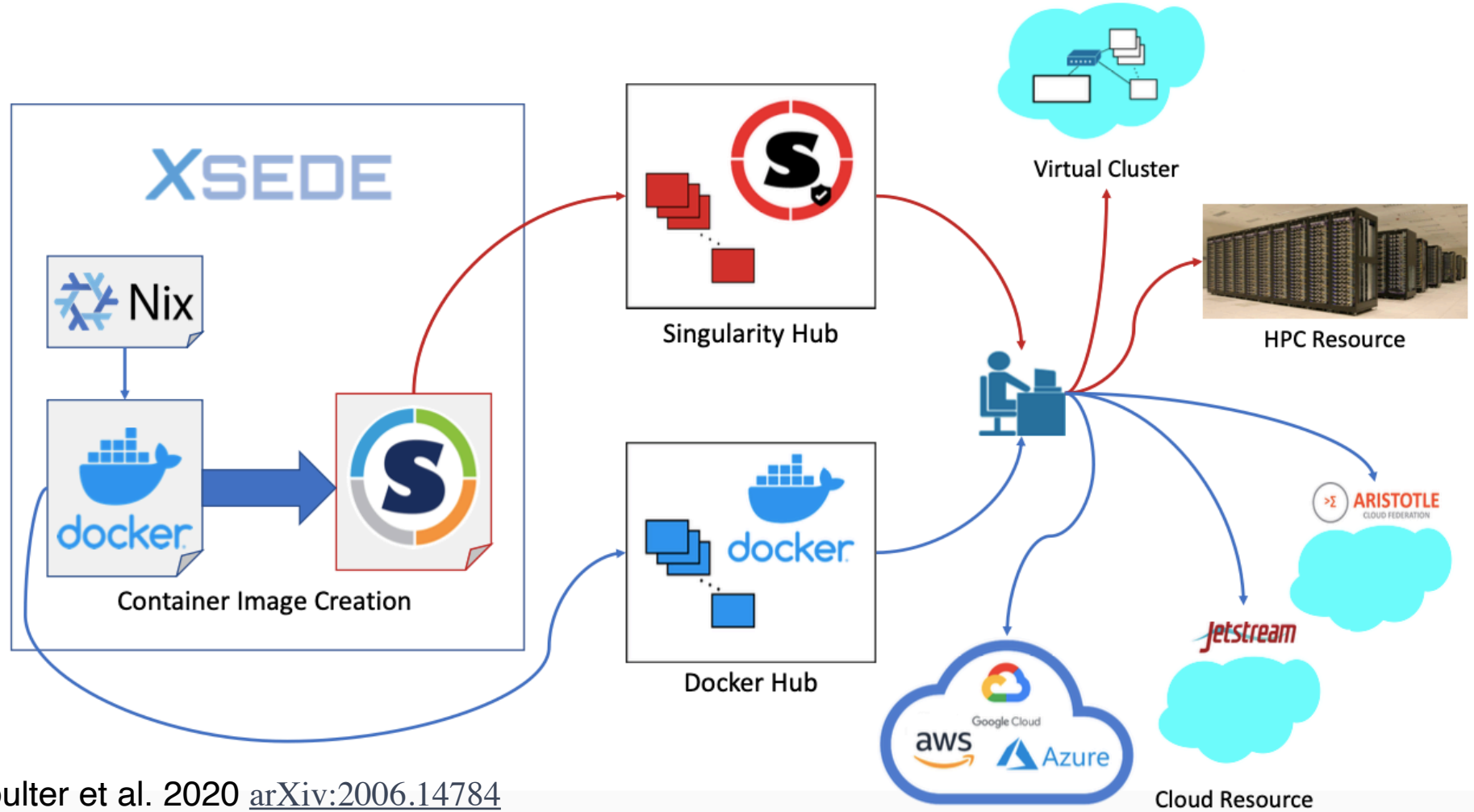
Security

Cloud VMs

- Implement security at a Virtual Machine (VM) level
  - Firewall
  - Security Groups
  - Limit ssh access
- For public images, pay attention to what they contain
  - Look for the Dockerfile
  - GitHub repo

Next Steps

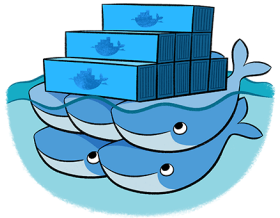
Reproducible Containers



Vaillancourt and Coulter et al. 2020 arXiv:2006.14784

Next Steps

Container Orchestration



+ ANSIBLE

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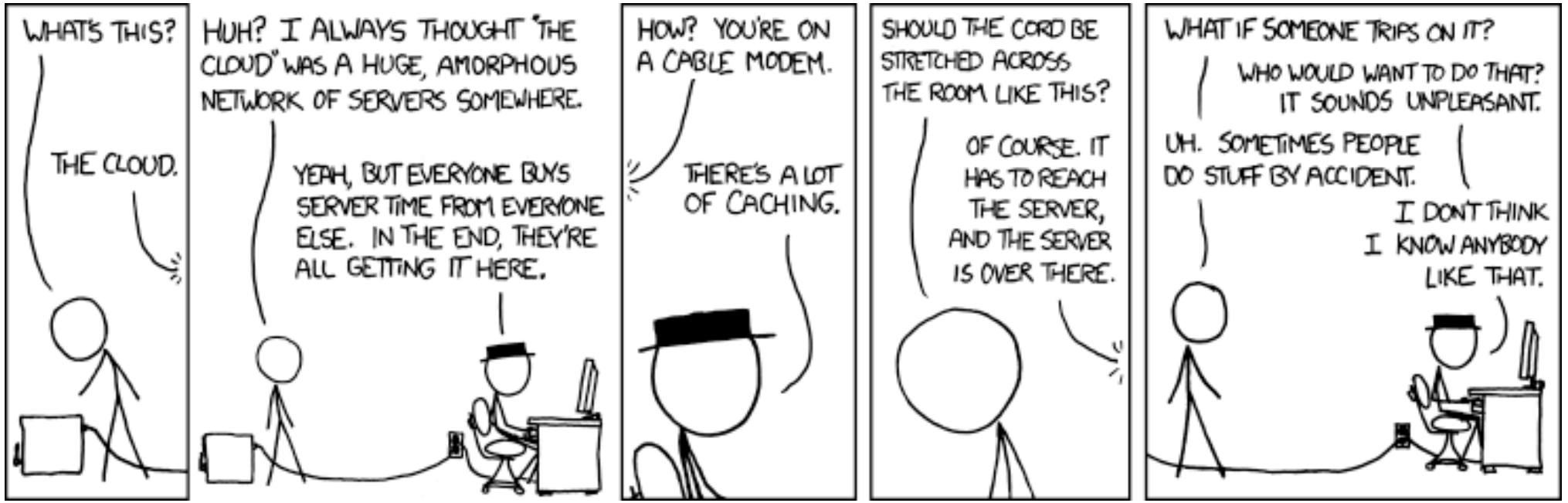
Questions?


WHAT'S THIS?
THE CLOUD.
HUH? I ALWAYS THOUGHT "THE CLOUD" WAS A HUGE, AMORPHOUS NETWORK OF SERVERS SOMEWHERE.
YEAH, BUT EVERYONE BUYS SERVER TIME FROM EVERYONE ELSE. IN THE END, THEY'RE ALL GETTING IT HERE.
HOW? YOU'RE ON A CABLE MODEM.
THERE'S A LOT OF CACHING.
SHOULD THE CORD BE STRETCHED ACROSS THE ROOM LIKE THIS?
OF COURSE. IT HAS TO REACH THE SERVER, AND THE SERVER IS OVER THERE.
WHAT IF SOMEONE TRIPS ON IT?
WHO WOULD WANT TO DO THAT? IT SOUNDS UNPLEASANT.
UH. SOMETIMES PEOPLE DO STUFF BY ACCIDENT.
I DON'T THINK I KNOW ANYBODY LIKE THAT.

Thank you!

https://github.com/XSEDE/Container_Tutorial

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