Cornell University

Containerization: Best Practices & Advanced Topics

Center for Advanced Computing (CAC)
Cornell University
XSEDE

XSEDE
Extreme Science and Engineering Discovery Environment

Containerization: Best Practices & Advanced Topics

Outline

- Lifecycle of a Container
  - Development vs Production
  - Reducing Container Sizes
  - Data Management
- Deploying a Container
  - Registries
  - In the Cloud
  - On a Shared Resource
- Security
- Next Steps
  - Reproducible Containers
  - Container Orchestration

Lifecycle of a Container

Containers for Development vs. Production

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

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

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

- 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

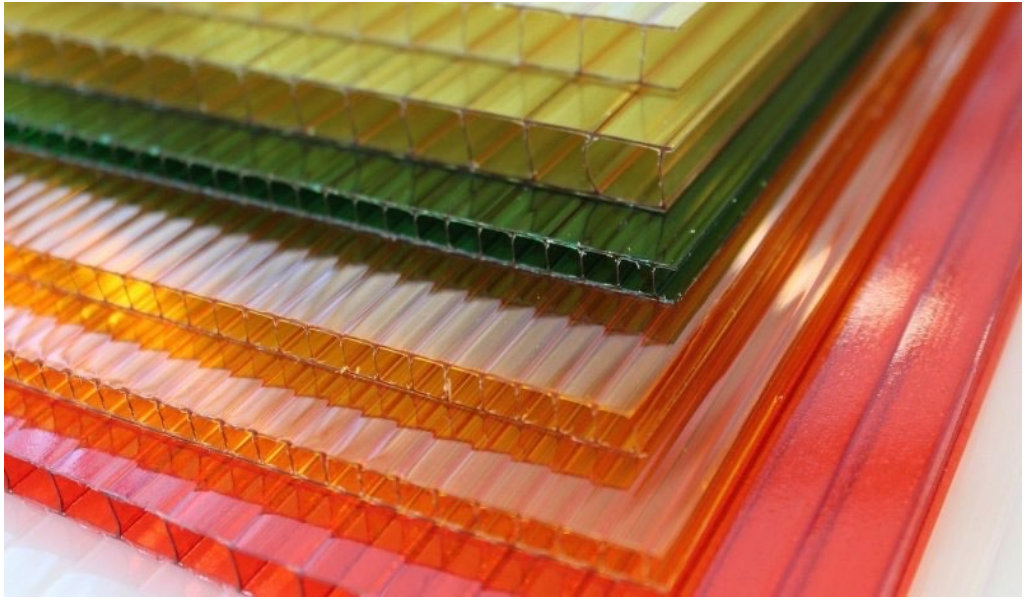
- Contains dependencies, code, environment variables, etc.
- Should be as lightweight as possible: no need for nice aesthetic features
- Code is static
- Requires a run script or easy commands

Lifecycle of a Container

Reducing Container Sizes

Docker Layers

- Base image
  - Rocky 205MB
  - Alma 189 MB
  - Debian 114MB
  - Ubuntu 73.9MB
  - Alpine 5.57MB

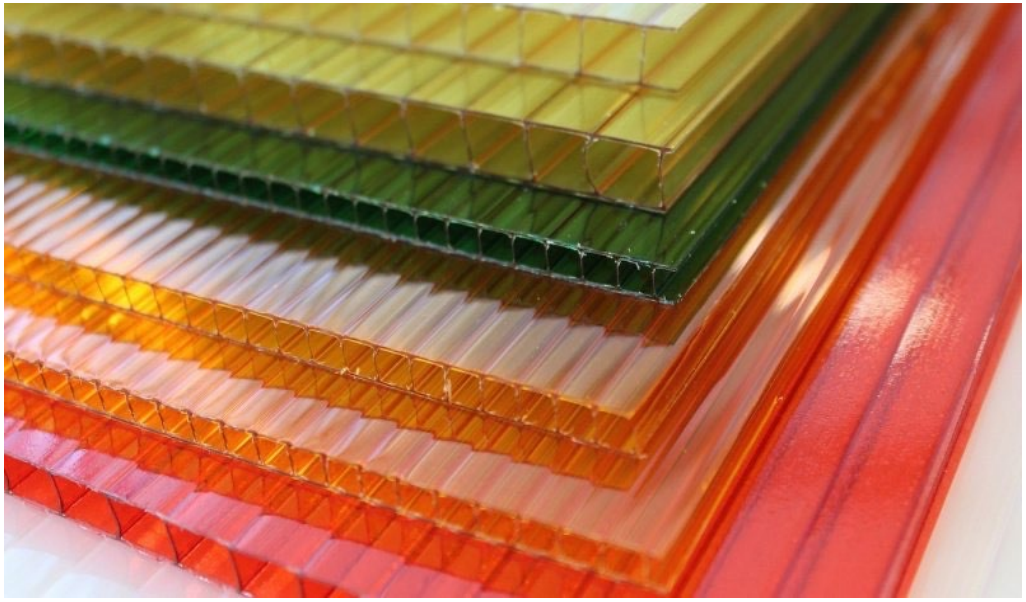


Lifecycle of a Container

Reducing Container Sizes

Docker Layers

- Base image
  - Rocky 205MB
  - Alma 189MB
  - 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

Example requirements.txt:

```
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, this is 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
- If using several RUN commands in a row, this is an opportunity to combine:

Use multi–stage builds

- Leverages docker build cache
- Can be used to remove some contents after the build for security

Lifecycle of a Container

Reducing Container Sizes

Combining multiple commands

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Don’t install what you don’t need

Multiple decoupled containers (microservices)

Lifecycle of a Container

Reducing Container Sizes

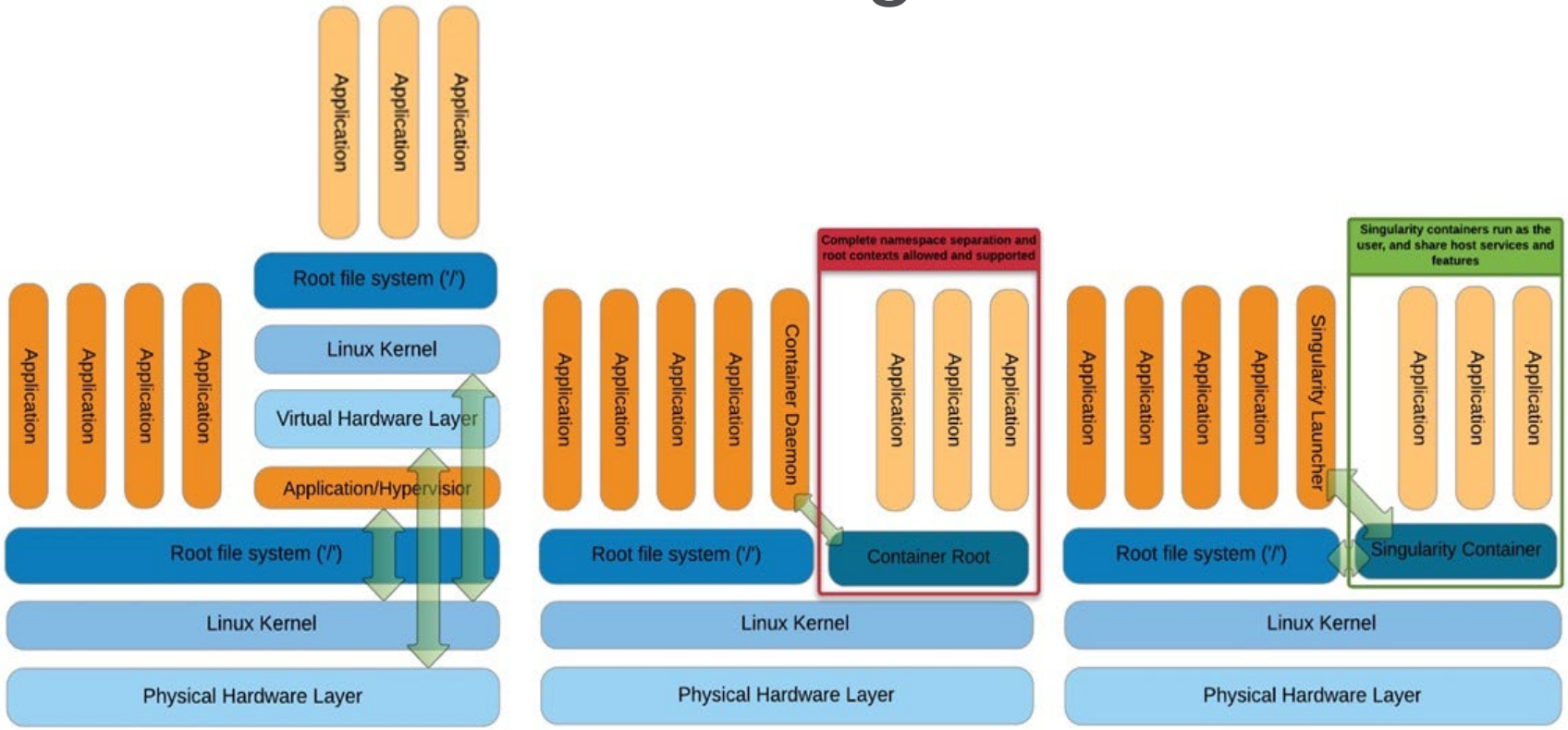
Using a prebuilt image from a registry?

- Decide whether to build your own
- Look at the layers to see what is excess
- Build files on GitHub can reveal unnecessary additions

Building your own is the best way to ensure you have only what you need

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

Deploying a Container

Uploading Containers

Containers on public registries can be a great way to

- Share scientific software portably
- Help others reproduce your research
- Create a community around a software/workflow
- Set up automated builds (connect your GitHub repo)

Common Public Registries

- DockerHub
- Sylabs Cloud Hosting (11GB limit)

Deploying a Container

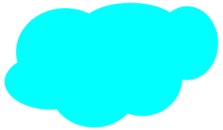
Best Practices for Uploading Containers

Don’t upload

- Private data – very important for research
- Private or licensed software

Do include

- Software licenses
- Documentation
- Software and dependencies
- Runscripts for production



Deploying a Container
In the Cloud

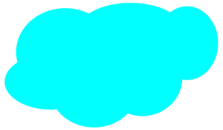
Will it work in the cloud?

- 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

Deploying a Container
In the Cloud



What is the right cloud?

- Private clouds using OpenStack have various options
- Public clouds have vendor-specific options galore
- Multi-cloud or generalized tools also available

Security is a consideration

Deploying a Container
On HPC Resources

Containers can simplify 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
- Automatic mounts for easy data access
- Multinode orchestration via Slurm

Job scripts and bind mounts may vary on different systems

Deploying a Container
On HPC Resources

Singularity with MPI

- MPI **major version** in the container *must* match the host
  https://sylabs.io/guides/3.5/user-guide/mpi.html
- Singlenode will work if MPI is run inside the container
- Multinode is more dependent on system
  - Choice of MPI library may be limited by hardware
  - Scheduler integrations, such as Slurm

Security

Root Access

- Sensitive and shared systems cannot allow root access
- XSEDE systems use Singularity
- Another option is Docker Rootless Mode
  - Docker Docs on Rootless Mode
  - DockerCon 2020 Talk on Rootless Mode
  - Recently became a fully supported feature
- Setup a user or users for shared Docker containers (same as shared system)

https://docs.docker.com/develop/develop-images/dockerfile_best-practices

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

Security

Other Security Features

Docker vulnerability scanning

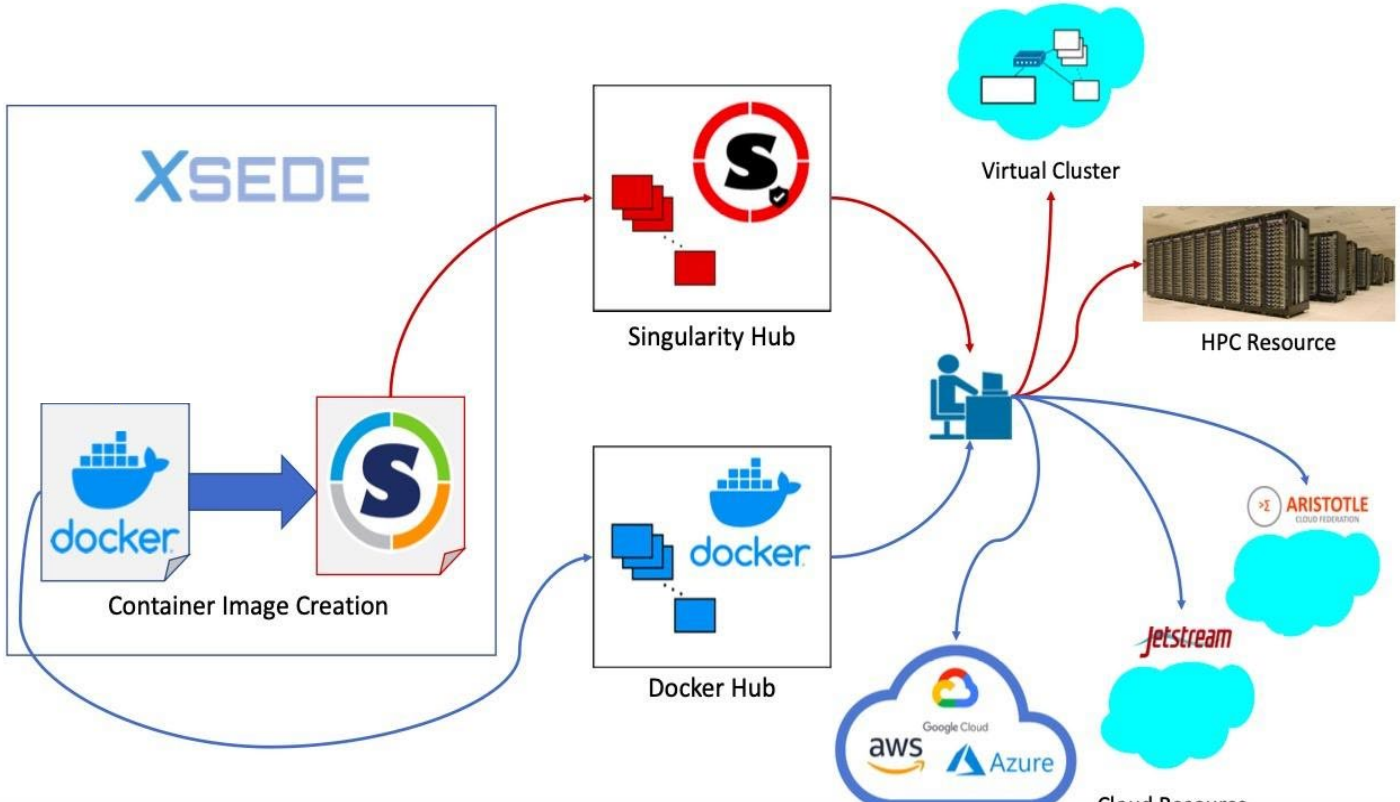
- https://docs.docker.com/engine/scan
- https://github.com/docker/scan-cli-plugin

Singularity Security Options

- Linux Capabilities
- Encrypted Containers
- https://sylabs.io/guides/3.5/user-guide/security_options.html#security-options

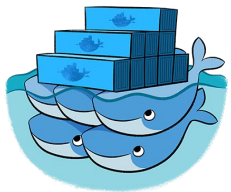
Next Steps

Reproducible Containers



Next Steps

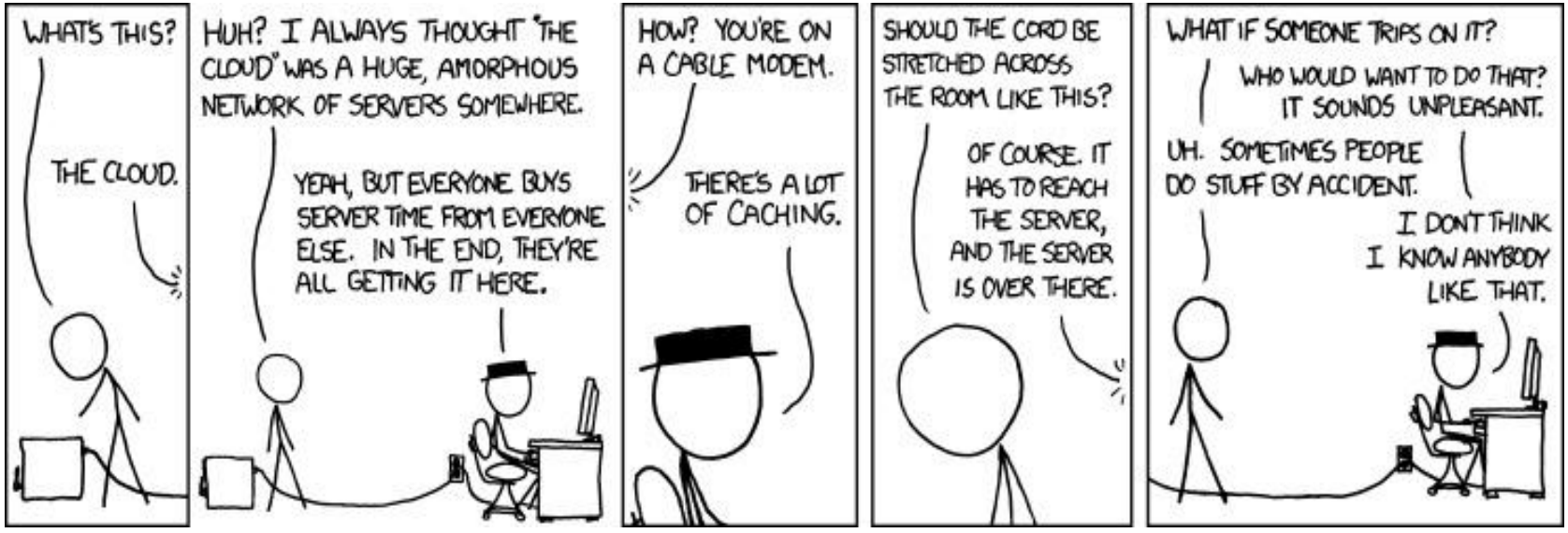
Container Orchestration



+

ANSIBLE

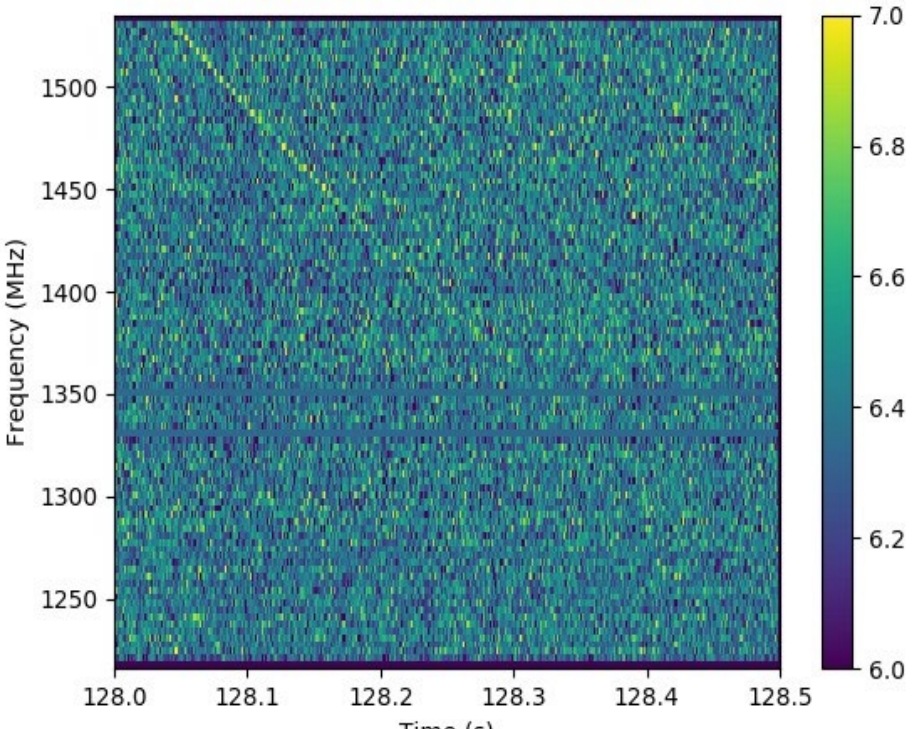
Questions?


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.


Cornell University
XSEDE
Extreme Science and Engineering Discovery Environment
Thank you!
https://github.com/XSEDE/Container_Tutorial
Center for Advanced Computing (CAC) Cornell University

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

Example Container: Radio Astronomy

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  - Based on jupyter/datascience-notebooks (includes Python, R, and more)
  - Wide variety of Radio Astronomy software and tools
- 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

Example Container: Radio Astronomy

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  - Based on jupyter/datascience-notebooks (includes Python, R, and more)
  - Wide variety of Radio Astronomy software and tools
- 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