

Peter Z. Vaillancourt
Computational Scientist,
Center for Advanced Computing (CAC)
Cornell University
XCRI Engineer, XSEDE





Docker to Singularity Conversion Different Philosophies

Docker

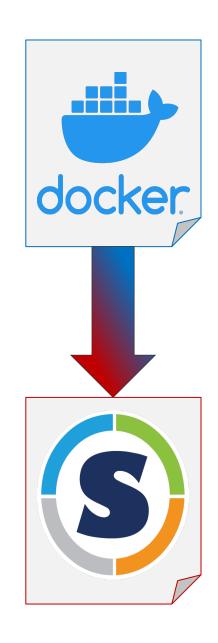
- Focus on flexibility and cloud usability
- Daemon runs as root
- Isolated from host filesystem
- Not originally designed for interoperability with Singularity or HPC systems

Singularity

- Focus on security and HPC usability
- Runs in userspace
- Direct Filesystem access
- Designed for interoperability with Docker

Overview of the Process

- 1. Create & Build the Dockerfile
- 2. Test the Docker container
- 3. Tag the Docker image and push to a DTR
- 4. Create the Singularity Definition file
- 5. Build & Test the Singularity container
- 6. (Optional) Push Singularity image to a registry





Docker to Singularity Conversion Where to Start?

FROM python:3.6-buster

SHELL ["/bin/bash", "-c"]

USER root

RUN apt-get update -y && \
apt-get install -y \
cmake \
liblapack-dev \
libblas-dev \
. . .

- Focus here is on the composition of the Dockerfile
 - For public images, find the Dockerfile where possible
 - Often available through Docker Hub links to GitHub repositories
 - Without the Dockerfile, you're taking a risk (security and conversion)
 - Keep these ideas in mind when building a Dockerfile
- Refer to Singularity Best Practices for Docker Images docs when attempting a conversion: https://sylabs.io/guides/3.5/user-guide/singularity_and_docker.html#best-practices

- 1. Account for differences in the trust model of Docker vs. Singularity
 - Do not create a user
 - Do not use the USER command unless it's to specify "USER root"

```
FROM python:3.6-buster
SHELL ["/bin/bash", "-c"]
USER root
RUN apt-get update -y && \
    apt-get install -y \
    cmake \
    liblapack-dev \
    libblas-dev \
```

- 1. Account for differences in the trust model of Docker vs. Singularity
 - Do not create a user
 - Do not use the USER command unless it's to specify "USER root"
- 2. Account for potential changes in the underlying Docker image
 - Use a Singularity definition file to pull and convert
 - Version pinning of Docker image can mitigate this, but not alleviate it entirely
 - Do a "diff" before "pull"
 - Also see: https://singularityhub.github.io/container-diff/

```
FROM python:3.6-buster
SHELL ["/bin/bash", "-c"]
USER root
RUN apt-get update -y && \
    apt-get install −y \
    cmake \
    liblapack-dev \
    libblas-dev \
```

Best Practices

3. Declare environment Variables in the Dockerfile

- Do not declare them in other files (i.e. .bashrc or .profile)
- Understand Singularity definition files:
 https://sylabs.io/guides/3.5/user-guide/definition_files.html#definitionfiles

```
RUN apt-get update -y && \
    apt-get install -y \
    cmake \
    liblapack-dev \
ENV PATH=$PATH:$PRESTO/bin
COPY file.py /root
```

Best Practices

3. Declare environment Variables in the Dockerfile

- Do not declare them in other files (i.e. .bashrc or .profile)
- Understand Singularity definition files: <u>https://sylabs.io/guides/3.5/user-guide/definition_files.html#definitionfiles</u>

4. Avoid installing to "/root"

- Not a blanket ban, but can sometimes cause issues
- User access remains the same as on host
- Cannot make changes to the read-only filesystem

```
RUN apt-get update -y && \
    apt-get install -y \
    cmake \
    liblapack-dev \
ENV PATH=$PATH:$PRESTO/bin
COPY file.py /root
```

Best Practices

5. Prepare for "/" to be read-only

- Overlay FS can allow changes, but not allowed on some HPC systems: https://sylabs.io/guides/3.5/user-guide/persistent_overlays.html
- The default install locations of most trusted/maintained software will just work
- A good place to install may be a subdirectory of /opt or /usr/local

```
COPY file.py /root
ENV PATH=$PATH:$PRESTO/bin
COPY file.py $HOME
COPY file2.py $TMP
RUN 1dconfig
```

- 5. Prepare for "/" to be read-only
 - Overlay FS can allow changes, but not allowed on some HPC systems: https://sylabs.io/guides/3.5/user-guide/persistent_overlays.html
 - The default install locations of most trusted/maintained software will just work
 - A good place to install may be a subdirectory of /opt or /usr/local
- 6. Avoid placing files in "\$HOME" or "\$TMP"

```
COPY file.py /root
ENV PATH=$PATH:$PRESTO/bin
COPY file.py $HOME
COPY file2.py $TMP
RUN 1dconfig
```

- 5. Prepare for "/" to be read-only
 - Overlay FS can allow changes, but not allowed on some HPC systems: https://sylabs.io/guides/3.5/user-guide/persistent_overlays.html
 - The default install locations of most trusted/maintained software will just work
 - A good place to install may be a subdirectory of /opt or /usr/local
- 6. Avoid placing files in "\$HOME" or "\$TMP"
- 7. Ensure symbolically linked libraries are cached
 - Can run "Idconfig" at or near the end of the Dockerfile

```
COPY file.py /root
ENV PATH=$PATH:$PRESTO/bin
COPY file.py $HOME
COPY file2.py $TMP
RUN 1dconfig
```

Best Practices

8. Do not use plain text passwords

 Can use the "--docker-login" option for Singularity "pull" and "build" commands

```
Bootstrap: docker
From: xsede/centos-nix-
base:latest
%runscript
    exec echo "Hello!"
%test
    grep -q NAME=\"CentOS\
Linux\" /etc/os-release
```

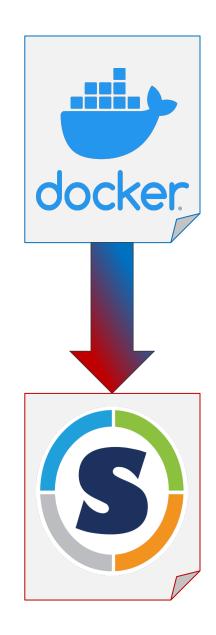
- 8. Do not use plain text passwords
 - Can use the "--docker-login" option for Singularity "pull" and "build" commands
- 9. Use the "%runscript" environment to execute commands in the container
 - Removes ambiguity

```
Bootstrap: docker
From: xsede/centos-nix-
base:latest
%runscript
    exec echo "Hello!"
%test
    grep -q NAME=\"CentOS\
Linux\" /etc/os-release
```

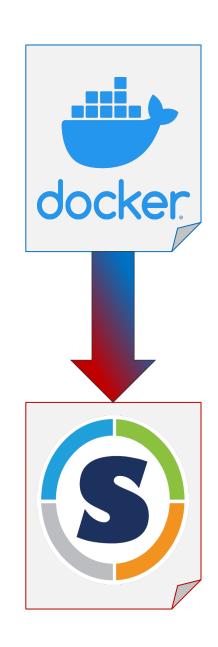


- DO run commands entirely as the root user in your Dockerfile
- DO a diff on the base image before building a new image of your container
- DO use the ENV directive for environment variables
- DO install to a subdirectory of /opt or /usr/local (recommended)
- DO run "Idconfig" near the end of your Dockerfile
- DO protect secure information

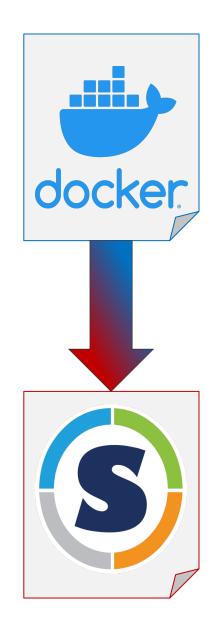
- 1. Dockerfile: https://github.com/federatedcloud/docker-PRESTO/blob/master/Dockerfile
 - docker build ...



- 1. Dockerfile: https://github.com/federatedcloud/docker-PRESTO/blob/master/Dockerfile
 - docker build ...
- 2. Test the Docker container
 - docker image
 - docker run <image> <command>
 - Or docker run --name=<name> <image> sleep 1000000 & docker exec --it <name> /bin/bash



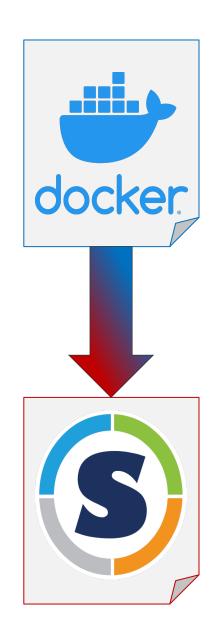
- 3. Tag the Docker image and push to a DTR
 - docker tag <image> <org/repo:tag>
 - docker push <org/repo:tag>



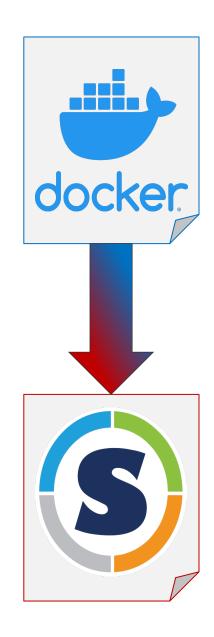
Example Completed Conversion

- 3. Tag the Docker image and push to a DTR
 - docker tag <image> <org/repo:tag>
 - docker push <org/repo:tag>
- 4. Singularity Definition file:

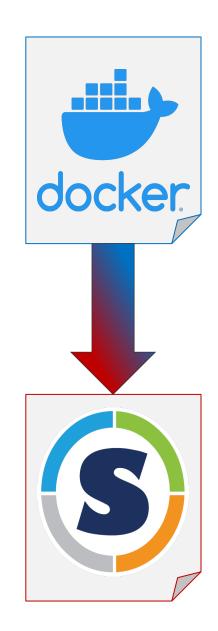
https://github.com/federatedcloud/singularity-PRESTO/blob/master/Singularity



- 5. Build & Test the Singularity container
 - singularity build ...

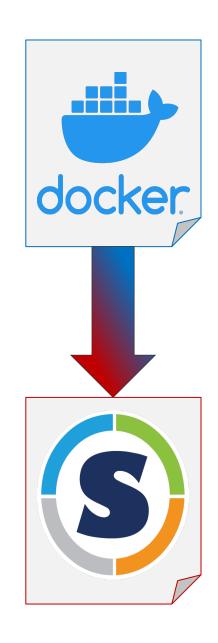


- 5. Build & Test the Singularity container
 - singularity build ...
- 6. (Optional) Push Singularity image to a registry



Overview of the Process

- 1. Create & Build the Dockerfile
- 2. Test the Docker container
- 3. Tag the Docker image and push to a DTR
- 4. Create the Singularity Definition file
- 5. Build & Test the Singularity container
- 6. (Optional) Push Singularity image to a registry





Docker to Singularity Conversion Also See



- All Tier 1 XSEDE systems have Singularity, for versions see: https://portal.xsede.org/software#/
- If you need to troubleshoot the conversion, see: https://sylabs.io/guides/3.5/user-guide/singularity_and_docker.html#troubleshooting
- For other conversion tools, especially for non-Linux users, see: https://github.com/singularityhub/docker2singularity



XSEDE

Extreme Science and Engineering Discovery Environment

Now try it out for yourself!

https://github.com/XSEDE/Container_Tutorial



Peter Vaillancourt
Computational Scientist
Center for Advanced Computing (CAC)
Cornell University

