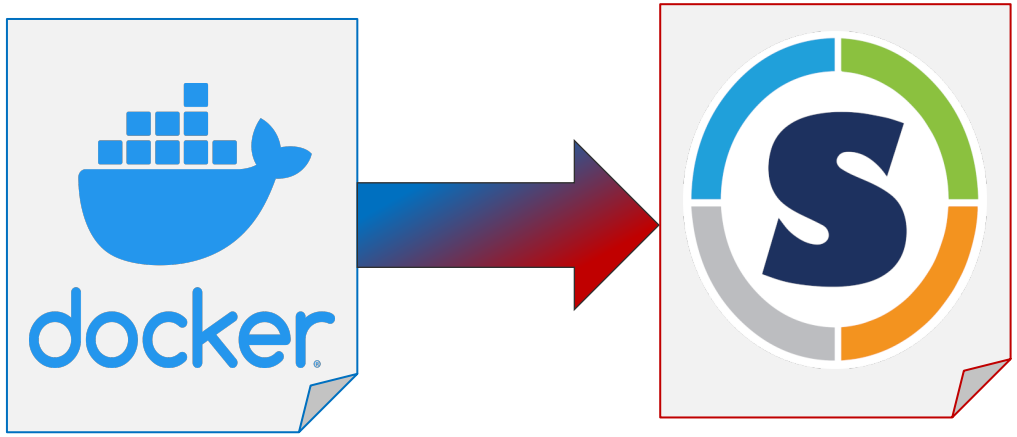

Docker to Singularity Conversion

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XSEDE
Extreme Science and Engineering Discovery Environment

Docker to Singularity Conversion

Different Philosophies

Docker

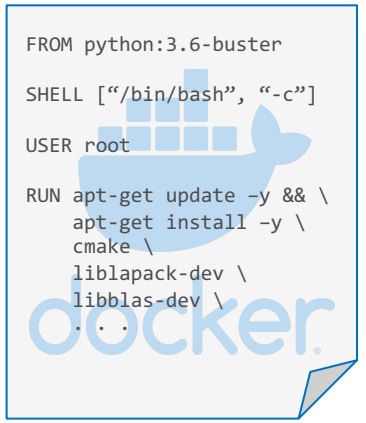
- Focus on flexibility and cloud usability
- Daemon runs as root
- Isolated from host filesystem
- Not originally designed for interoperability with Singularity or HPC systems

Singularity

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

Docker to Singularity Conversion

Where to Start?



- 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

Docker to Singularity Conversion

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 \
    . . .
```

Docker to Singularity Conversion

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"

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 \
    . . .
```

Docker to Singularity Conversion

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
. . .
```

Docker to Singularity Conversion

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

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
. . .
```

Docker to Singularity Conversion

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 ldconfig
```

Docker to Singularity Conversion

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
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6. Avoid placing files in “$HOME” or “$TMP”

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Docker to Singularity Conversion

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

6. Avoid placing files in “$HOME” or “$TMP”

7. Ensure symbolically linked libraries are cached
   - Can run “ldconfig” 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 ldconfig
```

Docker to Singularity Conversion

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
    . . .
```

Docker to Singularity Conversion

Best Practices

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
    . . .
```

Summary

- 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 “ldconfig” near the end of your Dockerfile
- DO protect secure information

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


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XSEDE
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Now try it out for yourself!
https://github.com/XSEDE/Container_Tutorial
docker
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