
WAYNE STATE
UNIVERSITY

Experiences Containerizing the JETSCAPE/XSCAPE Code

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Introduction

What is the JETSCAPE Collaboration?

The JETSCAPE Collaboration is an NSF funded multi-institutional effort to design the next generation of event generators to simulate the physics of ultra-relativistic heavy-ion collisions.

https://jetscape.org/

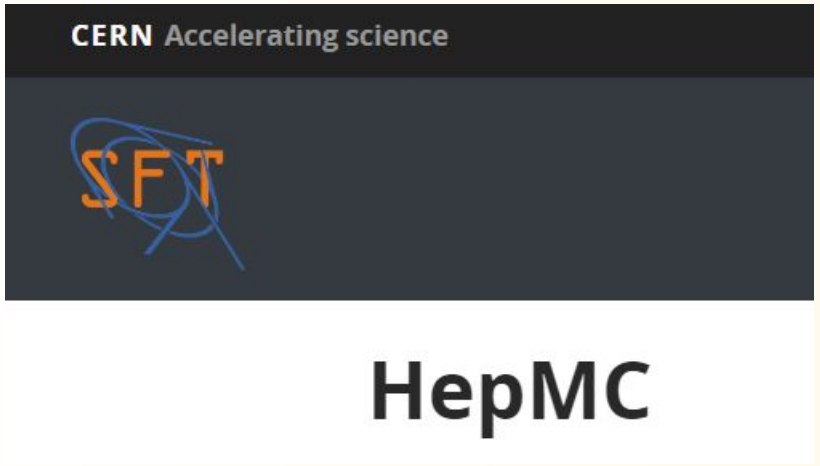
Introduction

JETSCAPE / X-SCAPE Docker Images

Often when software is containerized, the container executes the application as its entry-point.

```
ENTRYPOINT /bin/bash
```

JETSCAPE / X-SCAPE With Docker



https://ep-dep-sft.web.cern.ch/project/hepmc

https://pythia.org/

https://root.cern/

JETSCAPE / X-SCAPE With Docker

The **docker run** command mounts a folder from host system and users will install JETSCAPE or X-SCAPE in that mounted folder.

```
docker run -it -v ~/jetscape-docker:/home/jetscape-user --name myJetscape --user $(id -u):$(id -g) jetscape/base:stable
```

JETSCAPE / X-SCAPE With Docker

- Install Docker
- Clone JETSCAPE
- Start or Create the Container
- Build JETSCAPE
- Run JETSCAPE

https://github.com/JETSCAPE/JETSCAPE/wiki/Doc.Installation.Docker.Linux

JETSCAPE / X-SCAPE With Docker

```
# Clone X-SCAPE
RUN cd /home/jetscape-user \
&& git clone https://github.com/JETSCAPE/X-SCAPE.git

# Install External Packages
RUN cd /home/jetscape-user/X-SCAPE/external_packages \
&& ./get_music.sh \
&& ./get_iSS.sh \
&& ./get_freestream-milne.sh \
&& ./get_lbtTab.sh \
&& ./get_smash.sh \
&& ./get_3dglauber.sh \
&& cd /home/jetscape-user/X-SCAPE \
&& mkdir build \
&& cd build
```

Partial Dockerfile to create an image with the full installation of X-SCAPE.

```
# Build X-SCAPE
RUN cd /home/jetscape-user/X-SCAPE/build \
&& cmake .. -DCMAKE_CXX_STANDARD=14 -DUSE_ROOT=ON
-DUSE_3DGlauber=ON -DUSE_MUSIC=ON -DUSE_ISS=ON
-DUSE_FREESTREAM=ON -DUSE_SMASH=ON

RUN cd /home/jetscape-user/X-SCAPE/build \
&& make -j4
```

JETSCAPE / X-SCAPE With Singularity

Installing and Running on HPC Grids

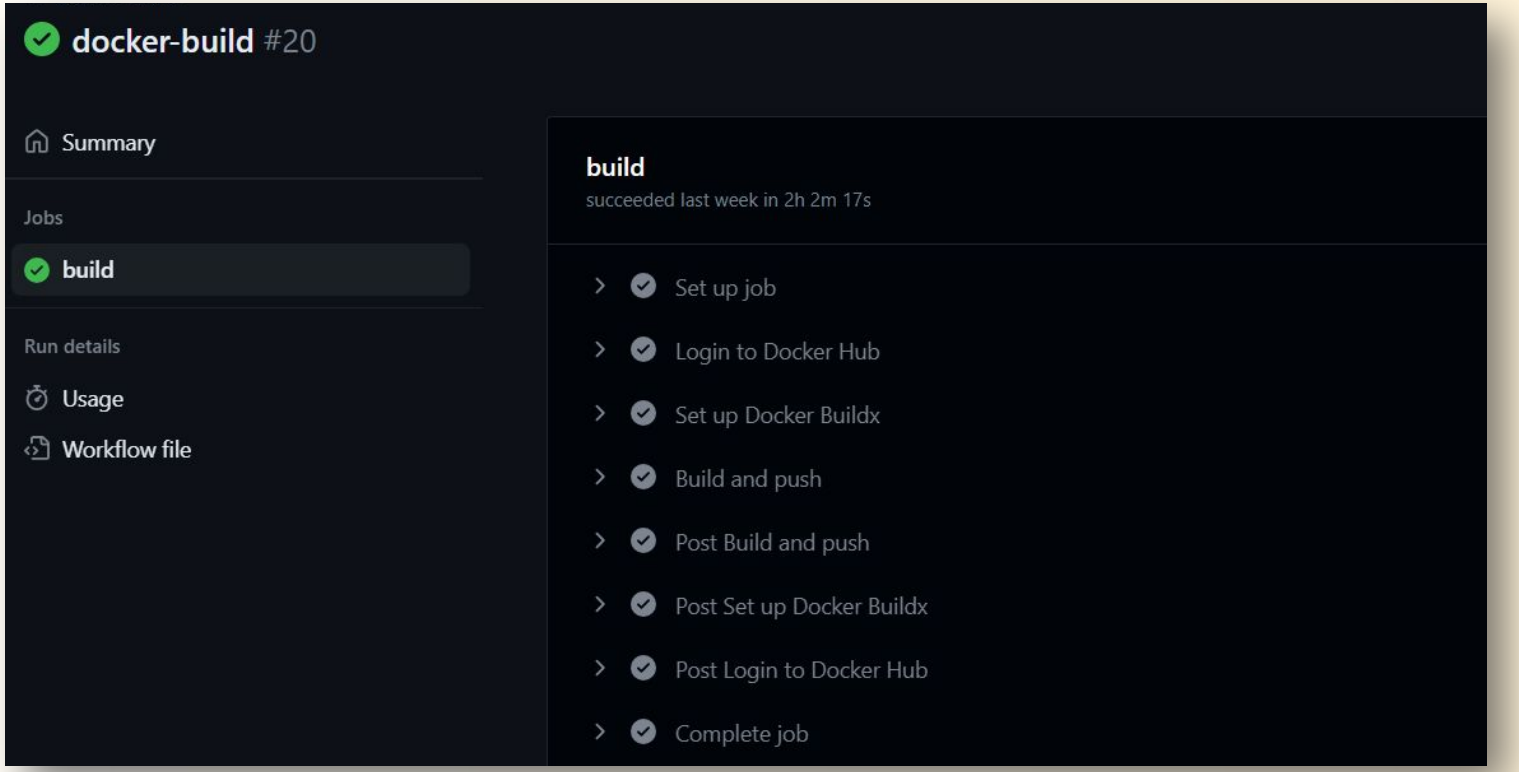
```
singularity build jet.sif docker://jetscape/base:stable
singularity shell jet.sif
cd /<path to your HPC account home folder>
mkdir jetscape
cd jetscape
git clone https://github.com/JETSCAPE/JETSCAPE.git
```

JETSCAPE / X-SCAPE Docker Dispatch

1. A Docker image with preinstalled dependencies.
2. A Docker image that includes a full installation of JETSCAPE.
3. A Docker image that includes a full installation of X-SCAPE.
4. A Docker image for Profiling and Optimization.
5. A Docker image for Rivet.
6. A Docker image for the JETSCAPE School.

A dispatch utility can help to automate the building and deployment of our several images.

JETSCAPE / X-SCAPE Docker Dispatch



https://github.com/JETSCAPE/TEST-EXAMPLES/actions/runs/5547934007/job/15028129286

JETSCAPE / X-SCAPE Multi-Architecture

```
steps:
  -
    name: Set up QEMU
    uses: docker/setup-qemu-action@v2
  -
    name: Set up Docker Buildx
    uses: docker/setup-buildx-action@v2
  -
    name: Login to Docker Hub
    uses: docker/login-action@v2
    with:
      username: ${{ secrets.DOCKER_USERNAME }}
      password: ${{ secrets.DOCKER_PASSWORD }}
  -
      name: Build and push
      uses: docker/build-push-action@v3
      with:
        file: ./docker/${{ inputs.path }}
        platforms: linux/arm64,linux/amd64
        push: true
        tags: ${{ secrets.DOCKER_USERNAME }}/${{
inputs.name }}:${{ inputs.version }}
```

A GitHub Actions Workflow file Using QEMU to build with ARM64/AMD64 Support

https://github.com/JETSCAPE/TEST-EXAMPLES/blob/main/.github/workflows/docker-arm.yaml

Summary

- JETSCAPE now provides several docker images and container environment for various use cases.
- Provides support for Singularity on HPC Grids.
- Uses GitHub Actions to Automate Deployment on Docker Hub.
- Uses QEMU to Provide Multi-Architecture Support (pre-release).

Summary

Thank You

Acknowledgements
The JETSCAPE Collaboration Members
https://jetscape.org/members.html

Summary

Discussion