

Singularity Containers and Comet Virtual Clusters

SDSC Summer Institute - 2017

Presented by Trevor Cooper

Review

- Access a node
- Examples
- Git Repositories

Access a Node

```
[etrain101@comet-ln2 ~]$ srun --pty --nodes=1 \  
--ntasks-per-node=24 -p compute -t 01:00:00 \  
--reservation=SI2017DAY2 --wait 0 /bin/bash
```

Examples

```
[etrain101@comet-ln2 ~]$ tree \  
/share/apps/examples/SI2017/Singularity
```

```
/share/apps/examples/SI2017/Singularity
```

```
|-- bootstrap.def
```

```
`-- singularity-hello-world
```

```
    |-- hello.sh
```

```
    |-- LICENSE
```

```
    |-- README.md
```

```
    `-- Singularity
```

1 directory, 5 files

Git Repository

```
[etrain101@comet-ln2 ~]$ git clone \  
https://github.com/hpcdevops/singularity-hello-world.git
```

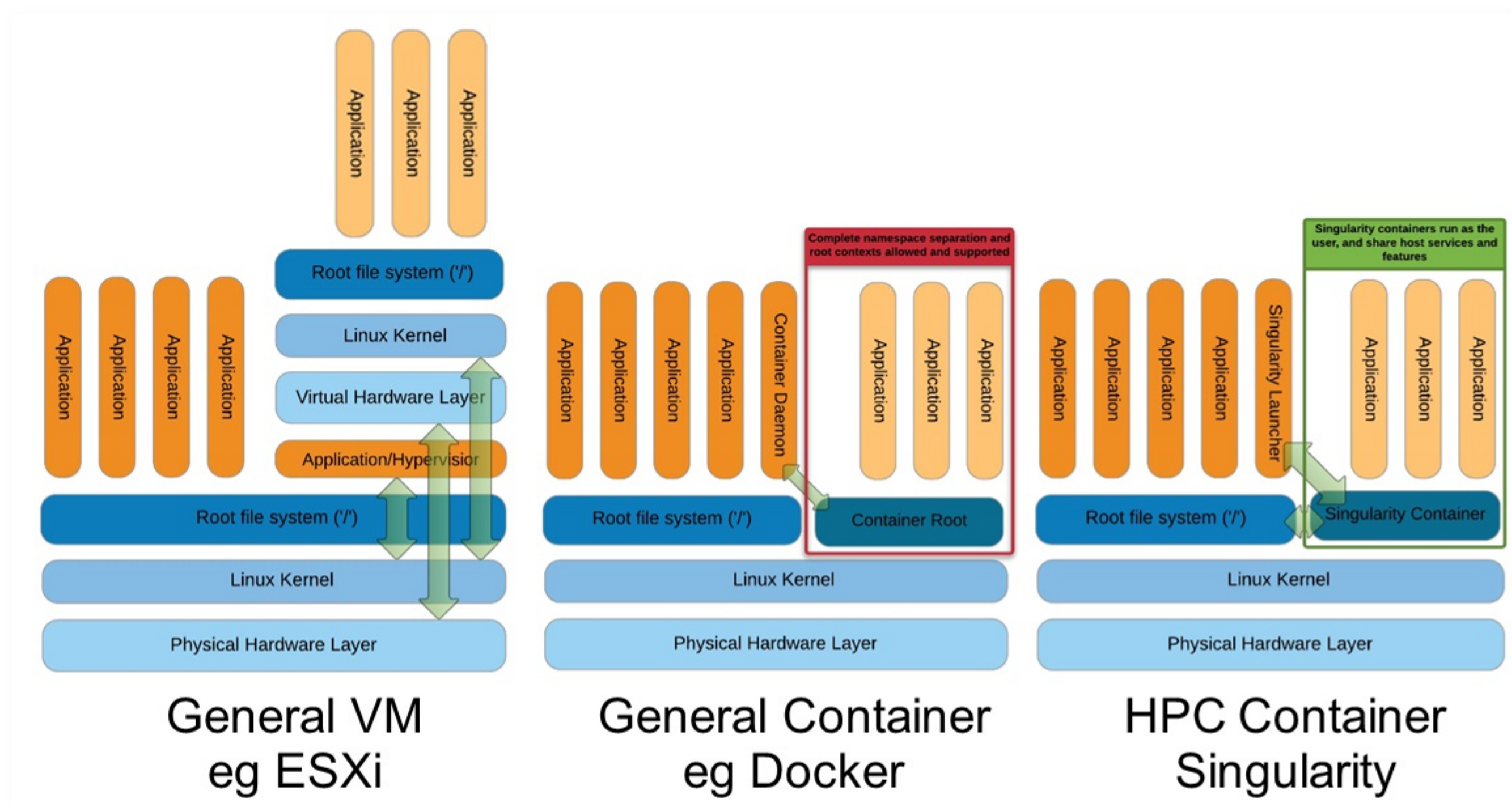
Overview

- Download & Install Singularity in VM
- Working with Singularity Containers
- Comet Virtual Clusters

Why Singularity?

```
COMMAND=apt-get -y install libx11-dev
COMMAND=apt-get install build-essential python-libdev
COMMAND=apt-get install build-essential openmpi-dev
COMMAND=apt-get install cmake
COMMAND=apt-get install g++
COMMAND=apt-get install git-lfs
COMMAND=apt-get install libXss.so.1
COMMAND=apt-get install libgdal1-dev libproj-dev
COMMAND=apt-get install libjsoncpp-dev libjsoncpp0
COMMAND=apt-get install libmpich-dev --user
COMMAND=apt-get install libpthread-stubs0 libpthread-stubs0-dev libx11-dev libx11-dev
COMMAND=apt-get install libudev0:i386
COMMAND=apt-get install numpy
COMMAND=apt-get install python-matplotlib
COMMAND=apt-get install python3
```

Why Singularity?



Singularity: Containers for Science, GM Kurtzer, 2017

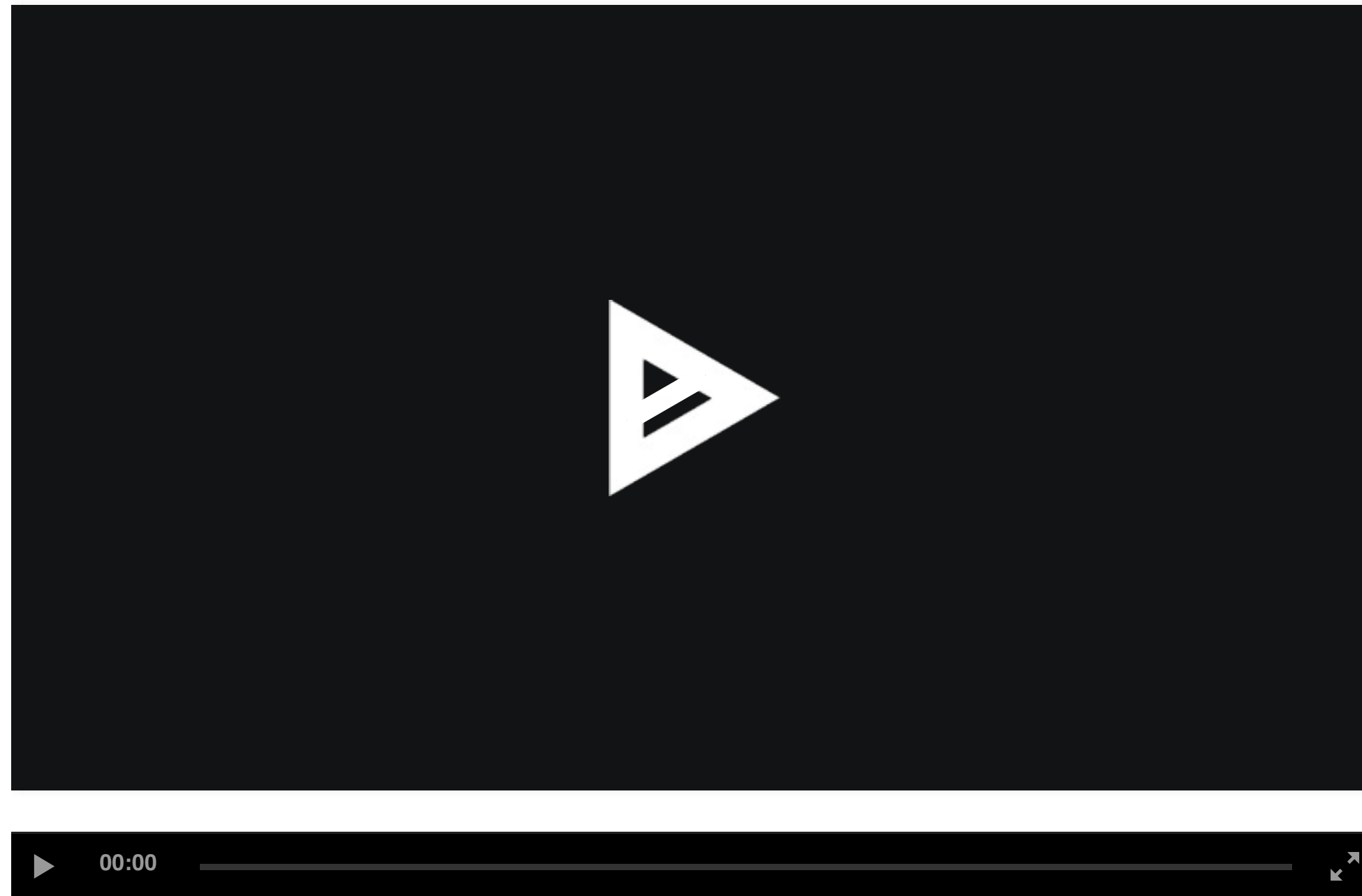
Download & Install Singularity

- Use a Virtual Machine...
- Download & Unpack Singularity
- Configure & Build Singularity
- Install & Test Singularity

Go to the Singularity website and download...

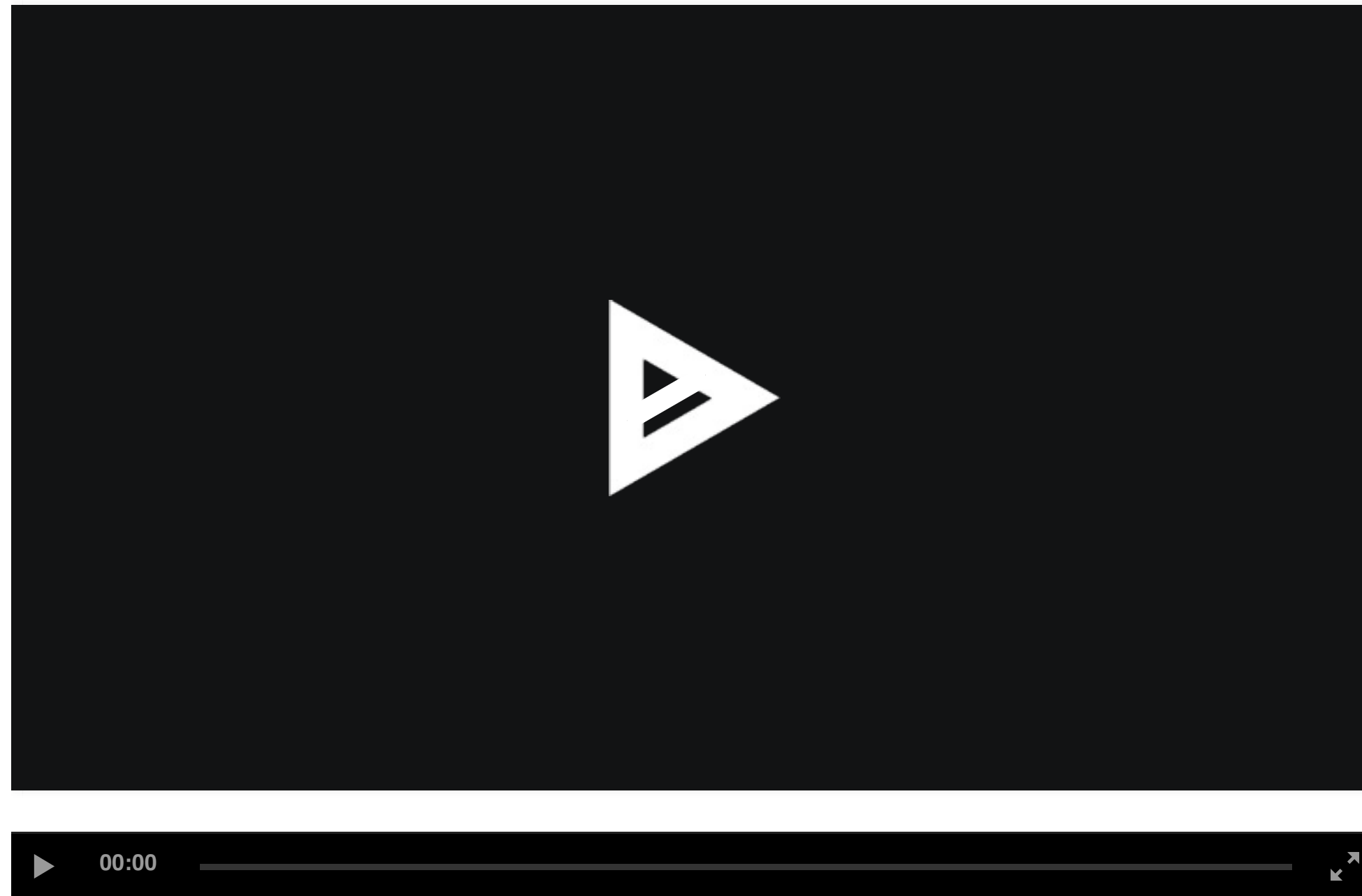
<http://singularity.lbl.gov/install-linux>

Download & Unpack Singularity



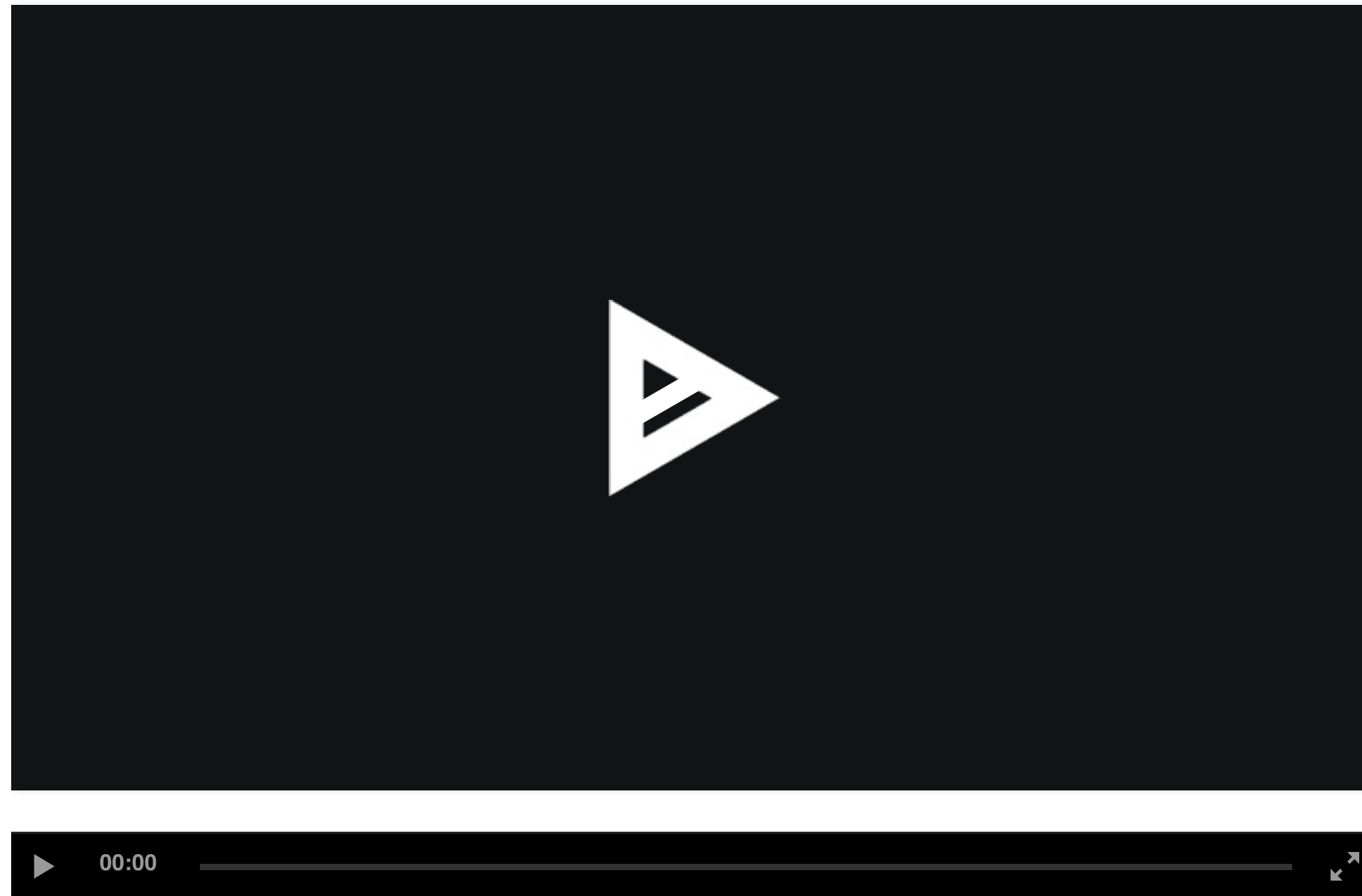
<https://asciinema.org/a/129866>

Configure & Build Singularity



<https://asciinema.org/a/129867>

Install & Test Singularity

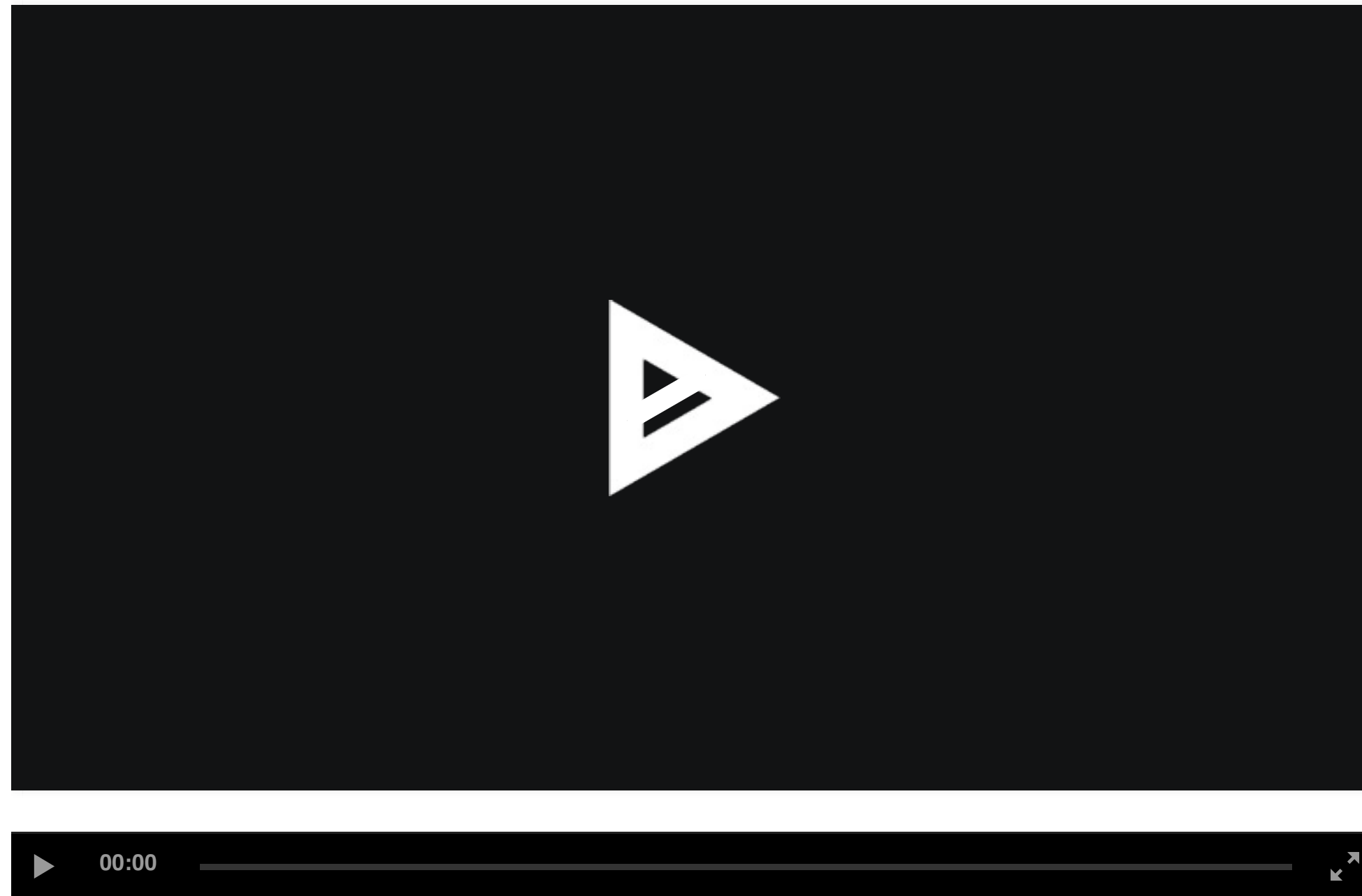


<https://asciinema.org/a/129868>

Building Singularity Containers

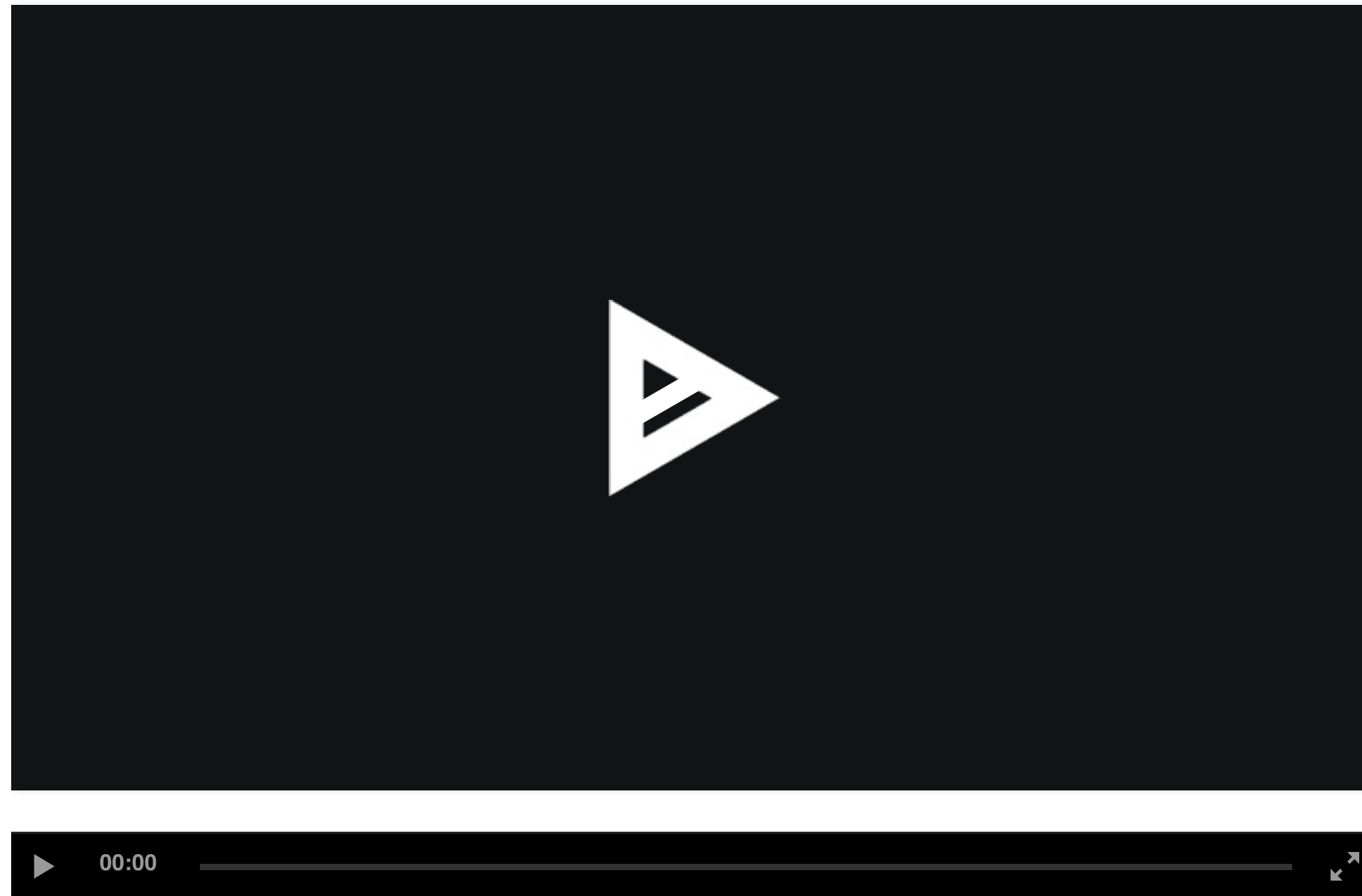
- Create Empty Container
- Import into Container
- Shell into Container
- Write into Container
- Bootstrap Container

Create Empty Container



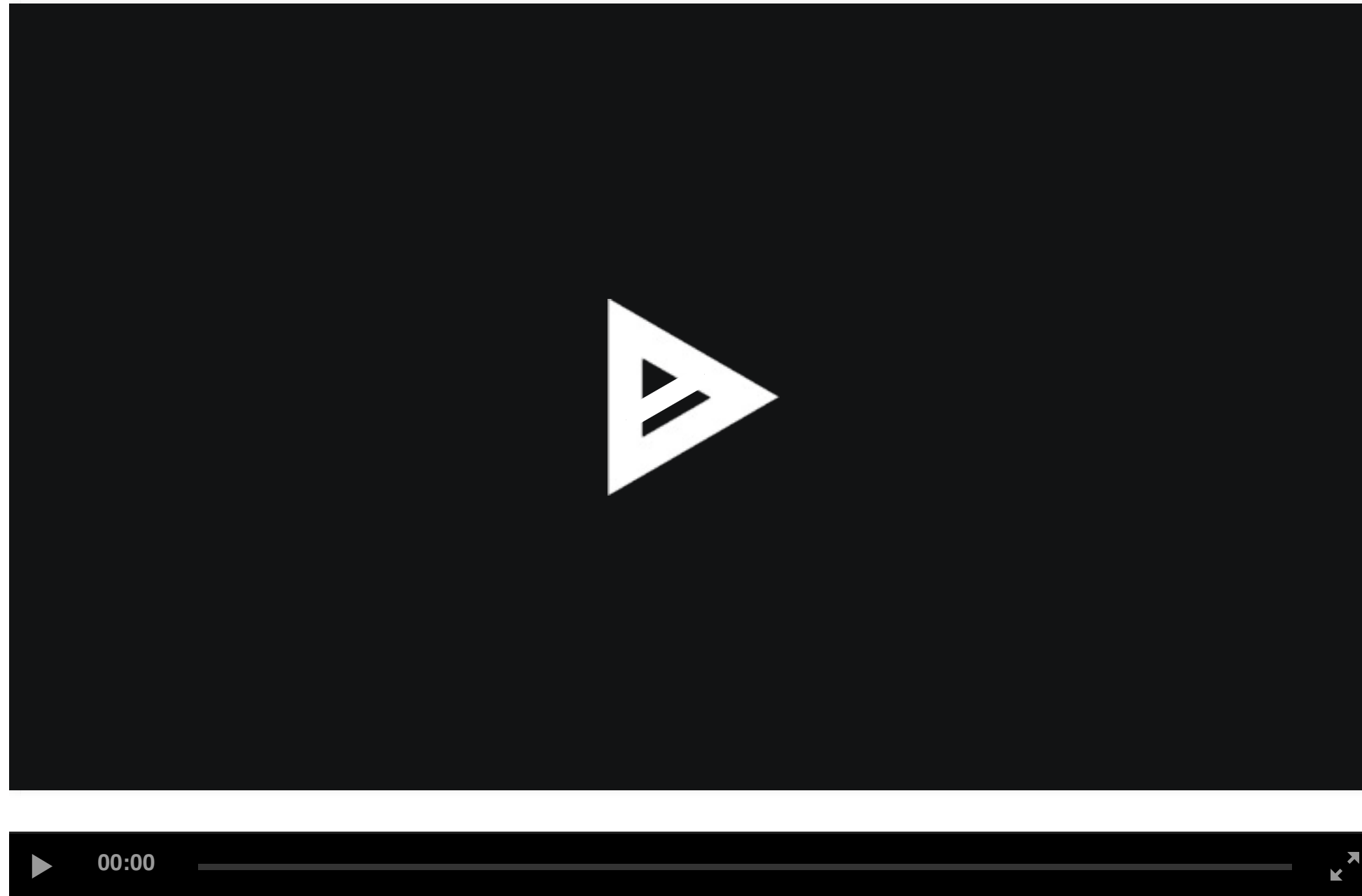
<https://asciinema.org/a/130106>

Import Into Container



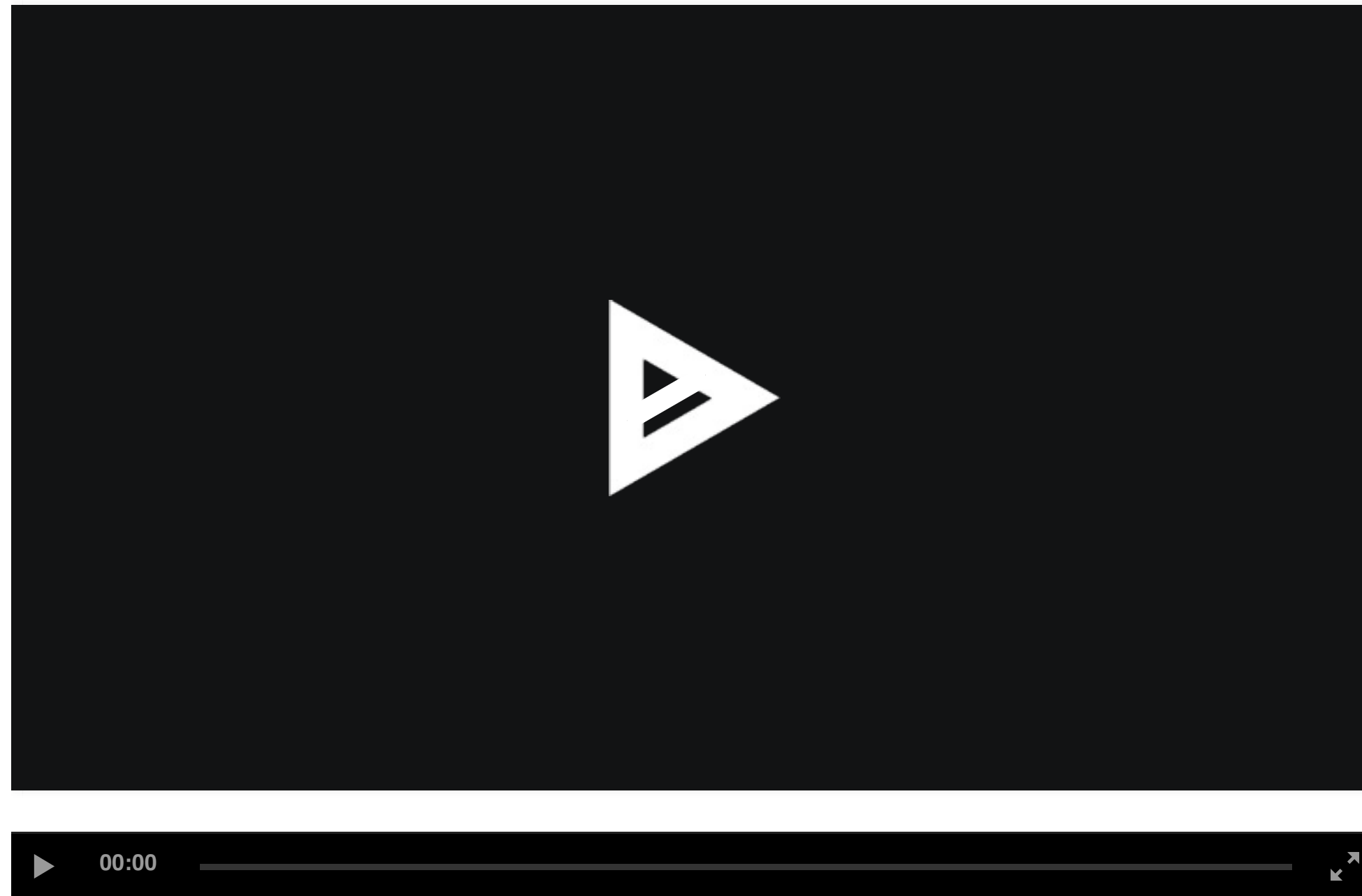
<https://asciinema.org/a/130107>

Shell into Container



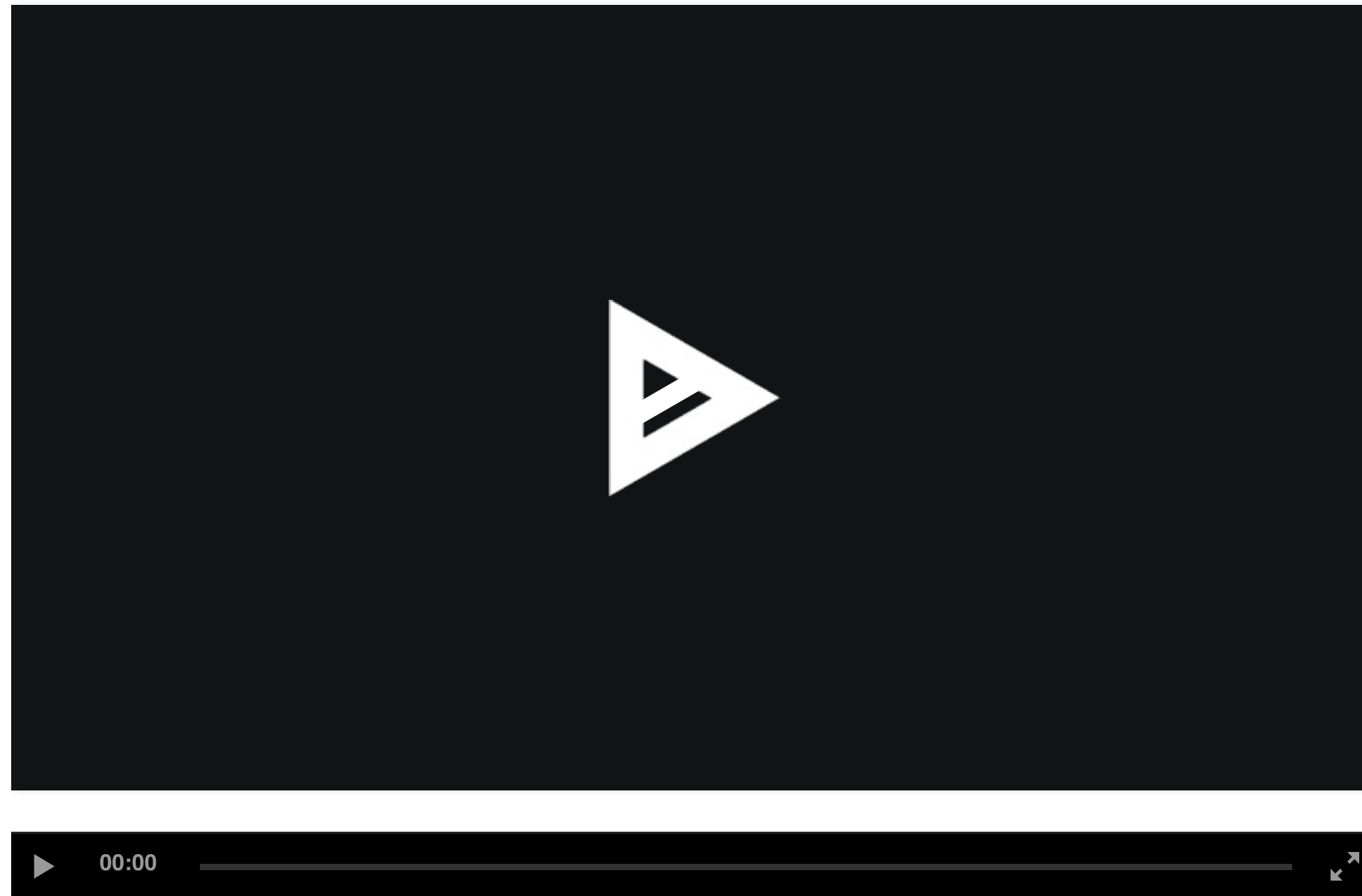
<https://asciinema.org/a/130109>

Write into Singularity Container



<https://asciinema.org/a/130110>

Bootstrap Container

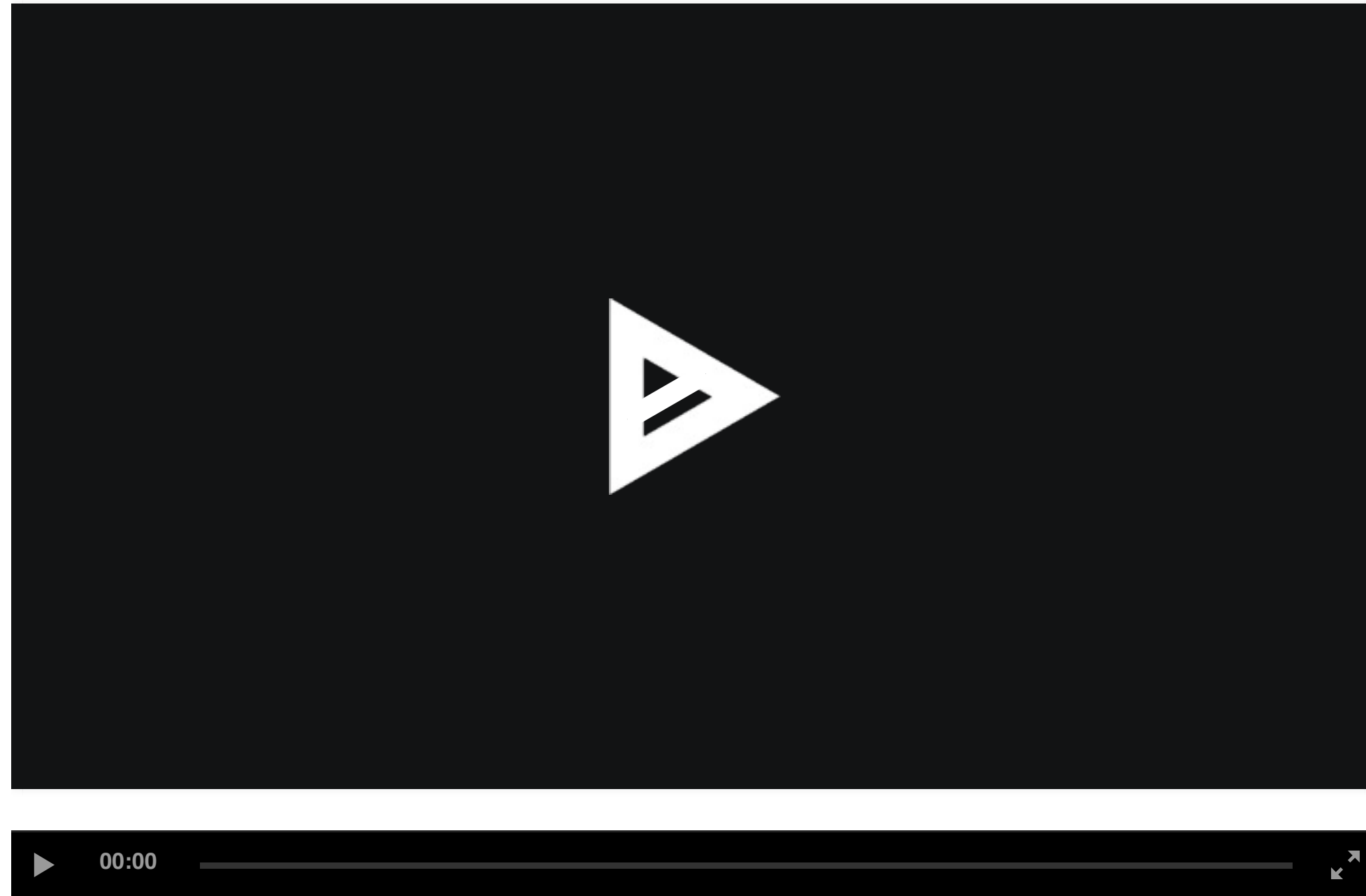


<https://asciinema.org/a/130111>

Running Singularity Containers on Comet

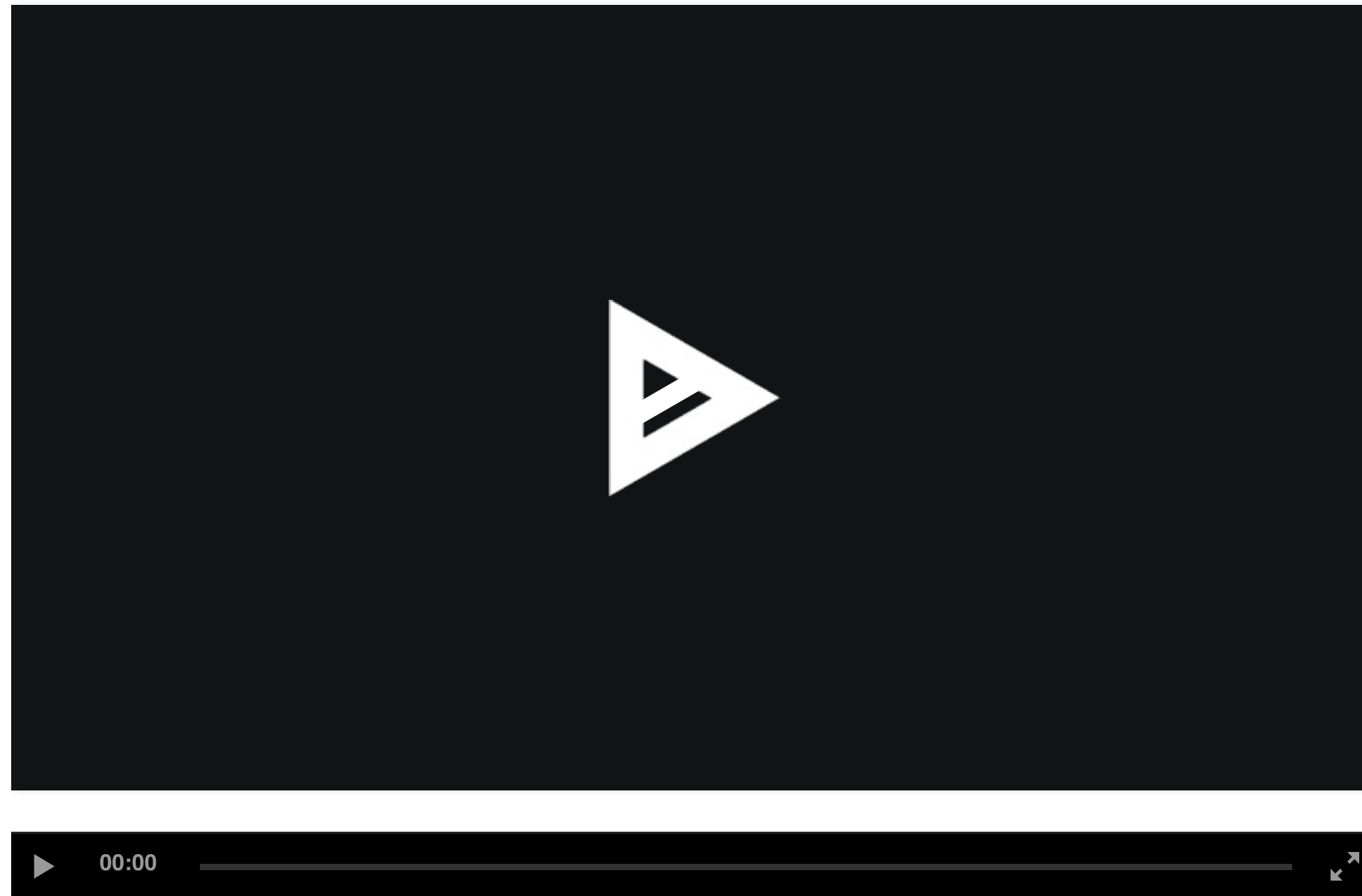
- Transfer Container to Comet
- Run Container on Comet
- Allocate Resources to Run Container
- Integrate Container with Slurm

Transfer Container to Comet



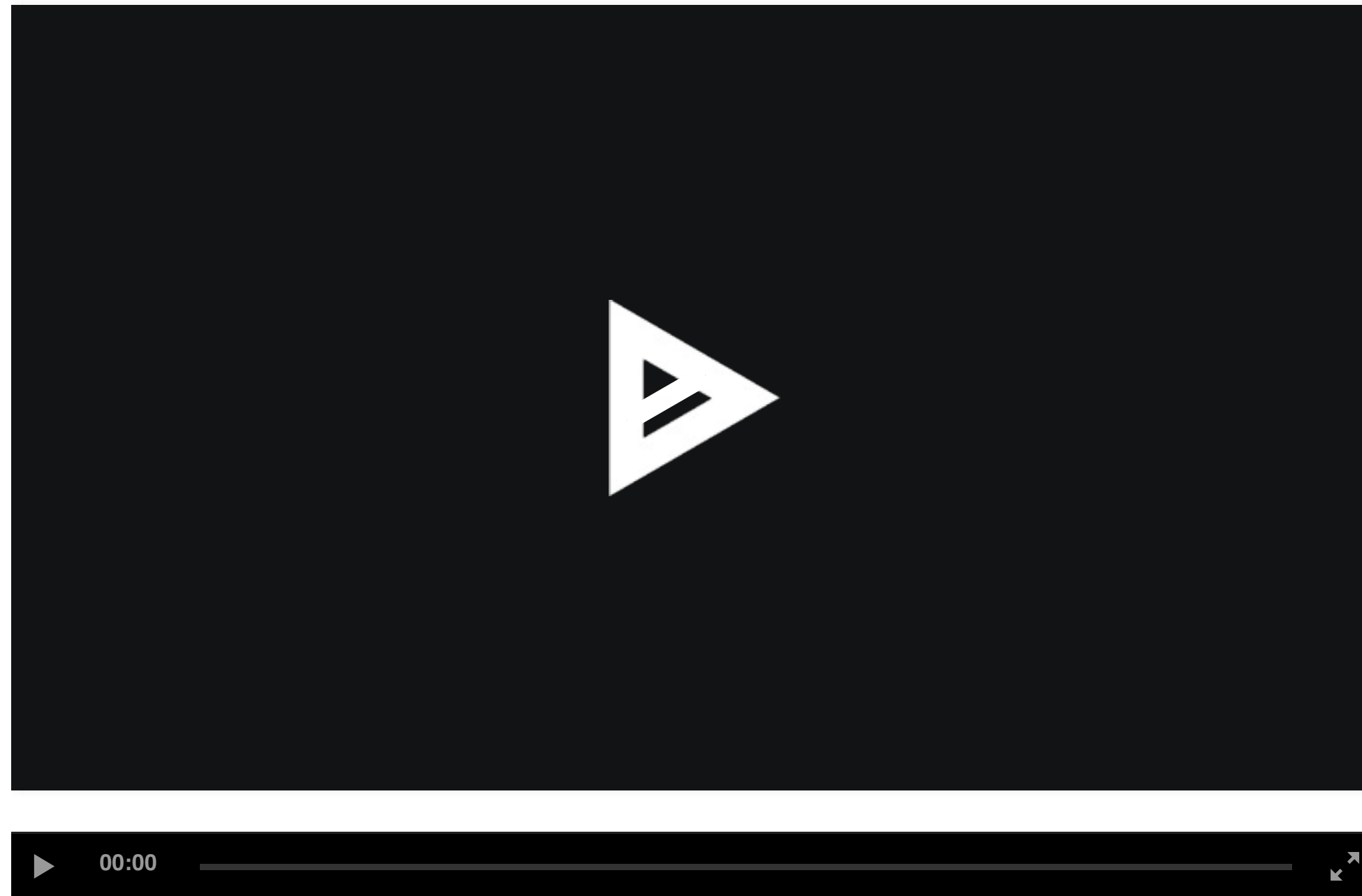
<https://asciinema.org/a/130195>

Run Container on Comet



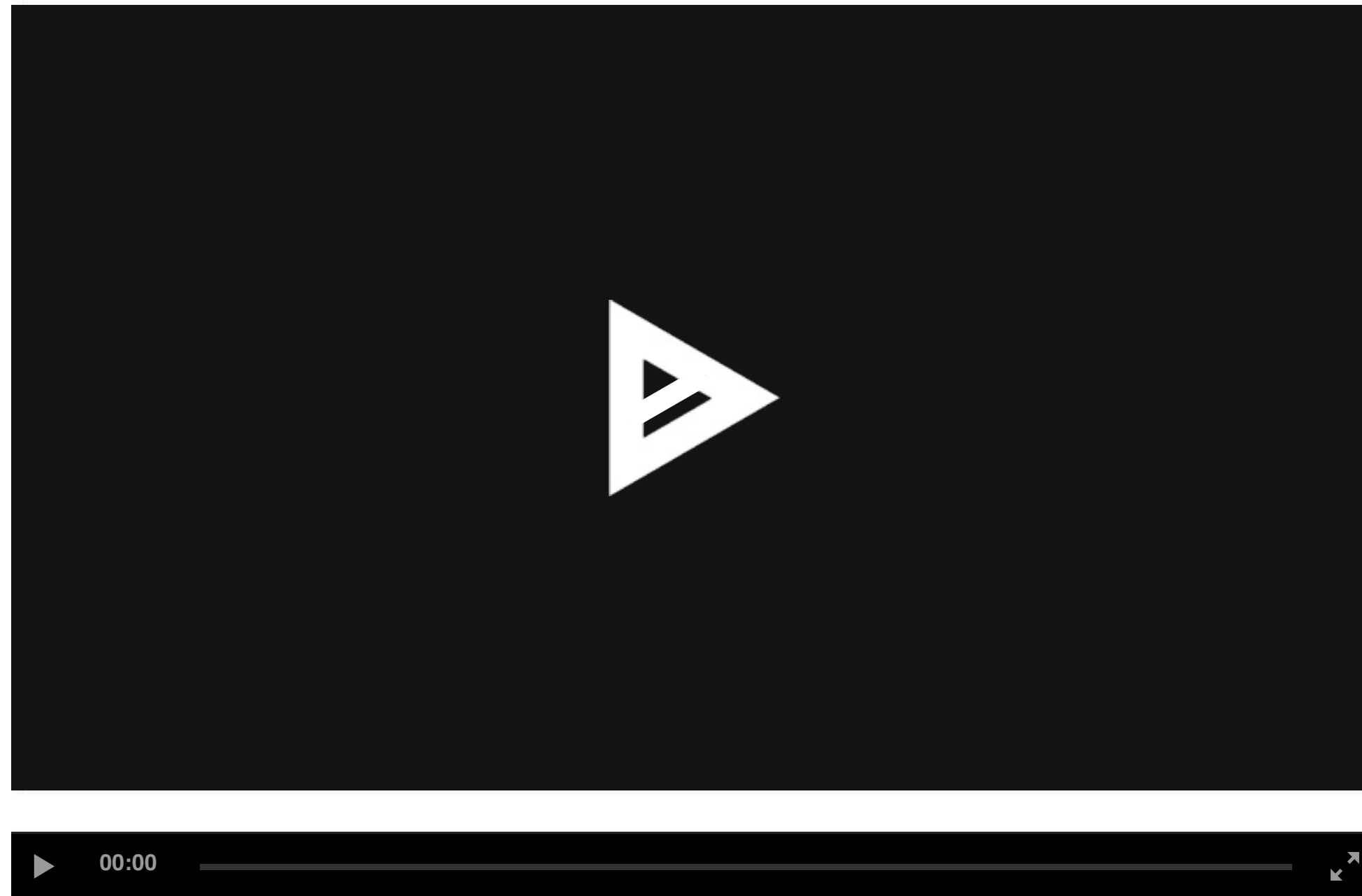
<https://asciinema.org/a/130196>

Allocate Resources to Run Container



<https://asciinema.org/a/130197>

Integrate Container with Slurm

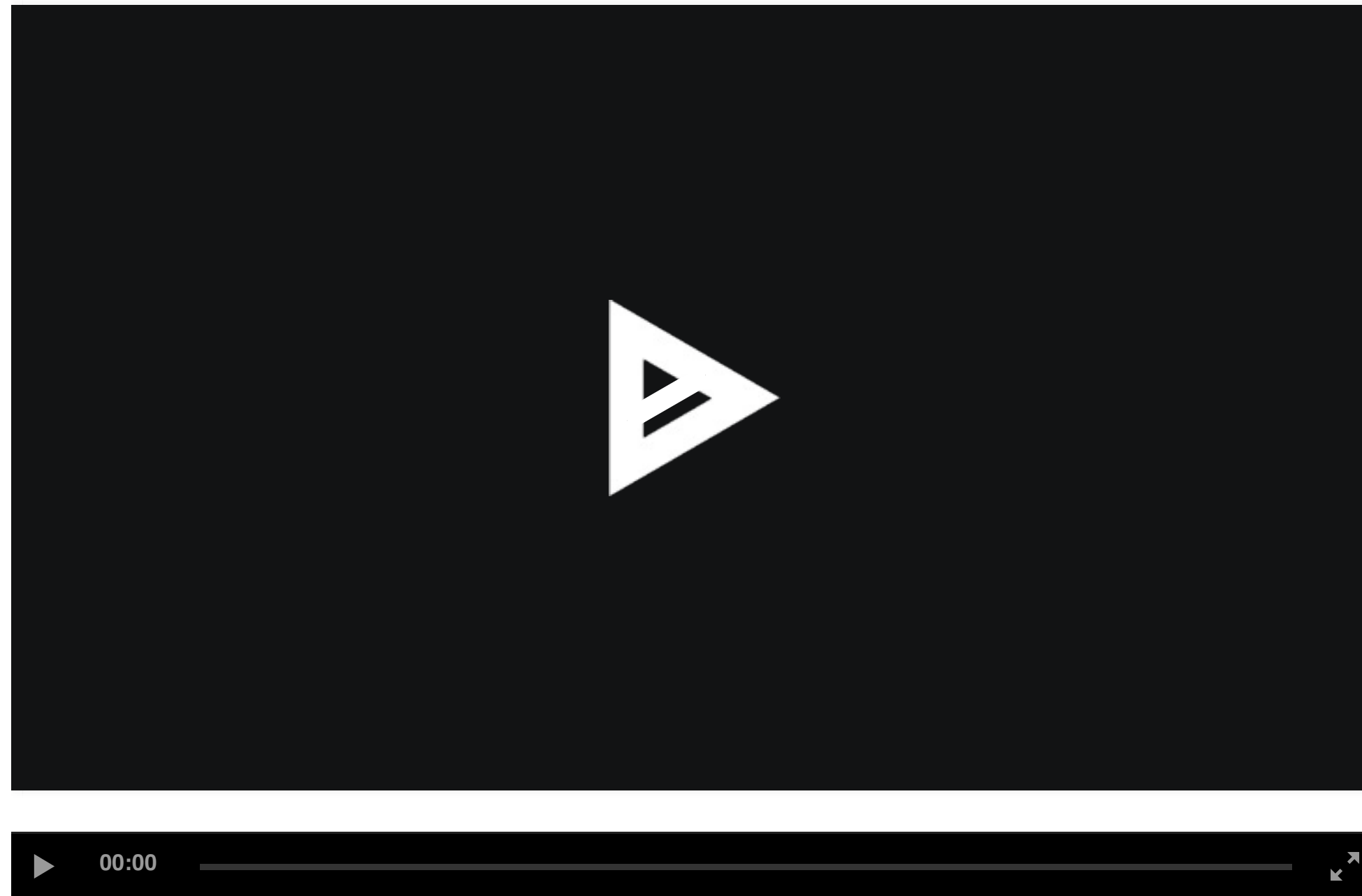


<https://asciinema.org/a/130218>

Is there an easier way?

- Pull Container Directly to Comet
- Remaining steps as before...

Pull Container Directly to Comet



<https://asciinema.org/a/129906>

Singularity Hub

- Build containers without a VM
- Share your science
- Prepare for Singularity Registry

<https://singularity-hub.org>

Build containers without a VM

- Definition in a Github repo...

The screenshot shows a web browser window displaying the GitHub repository page for `hpcdevops/singularity-hello-world`. The browser's address bar shows the repository name and a description: "Simple hello world container for Singularity". The GitHub navigation bar at the top includes the repository name, a search bar, and links for "Pull requests", "Issues", "Marketplace", and "Gist". On the right, there are notification and user profile icons.

Below the navigation bar, the repository name `hpcdevops / singularity-hello-world` is displayed, followed by buttons for "Watch", "Star", and "Fork", each with a count of 0. Below this is a tabbed interface with "Code" selected, and links for "Pull requests" (0), "Projects" (0), and "Insights".

The main heading is "Simple hello world container for Singularity". Below this, a summary bar shows "9 commits", "2 branches", "0 releases", and "1 contributor".

Below the summary bar, there are buttons for "Branch: master", "New pull request", "Create new file", "Upload files", "Find file", and a green "Clone or download" button.

The commit history is shown in a table:

| Commit | Message | Time |
|-----------------------------|---|------------------------------------|
| hpcdevops | Update README to include singularity pull command | Latest commit e5adfc2 17 hours ago |
| LICENSE | Initial commit | 9 days ago |
| README.md | Update README to include singularity pull command | 17 hours ago |
| Singularity | Minor formatting changes | 2 days ago |
| hello.sh | Import environment during bootstrap test | 2 days ago |

Build containers without a VM

- Definition in a Github repo...
- Automatically built on push...









SINGULARITYContainersAboutUser GuideTools

hpcdevops

hpcdevops/singularity-hello-world

DISCUSSIONMAKE PRIVATEBRANCHESEDIT BUILDERSDISABLE

Builds



| | Id ↓ | Tag | Build Date | Status | Version | |
|--------------------------|------|--------|---------------------------|----------|--|---|
| <input type="checkbox"/> | 1969 | master | July 20, 2017, 6:45 p.m. | COMPLETE | e5adfc2039340517130bfa8f187f3ef4d3870a27 |     ... |
| <input type="checkbox"/> | 1902 | master | July 19, 2017, 12:55 a.m. | COMPLETE | b50da388fc5892631d45bb8cf8a1dec3035bb58f |     ... |


Rows per page: 501 - 2 of 2

DELETE COLLECTION


Build containers without a VM

- Definition in a Github repo...
- Automatically built on push...
- Search, compare, etc...

SINGULARITY Containers About User Guide Tools  hpcdevops 

researchapps/tensorflow:cpu minus hpcdevops/tensorflow-gpu-nih:master 

Score: 0.6



Files

- libbfd-2.24-system.so
- libgirepository-1.0.so.1.0.0
- libopcodes-2.24-system.so
- libperl.so.5.18.2

Prepare for Singularity Registry

PEARC17 - Containers for Science (Slide 161) -
Vanessa Sochat

Comet Virtual Clusters

- Why use a Virtual Cluster?
- Installing Cloudmesh Client
- Running Cloudmesh Client

Why to use a Virtual Cluster?

- Require custom software we can't provide
- Require root access inside Comet
- Desire to expand local cluster to XSEDE resource

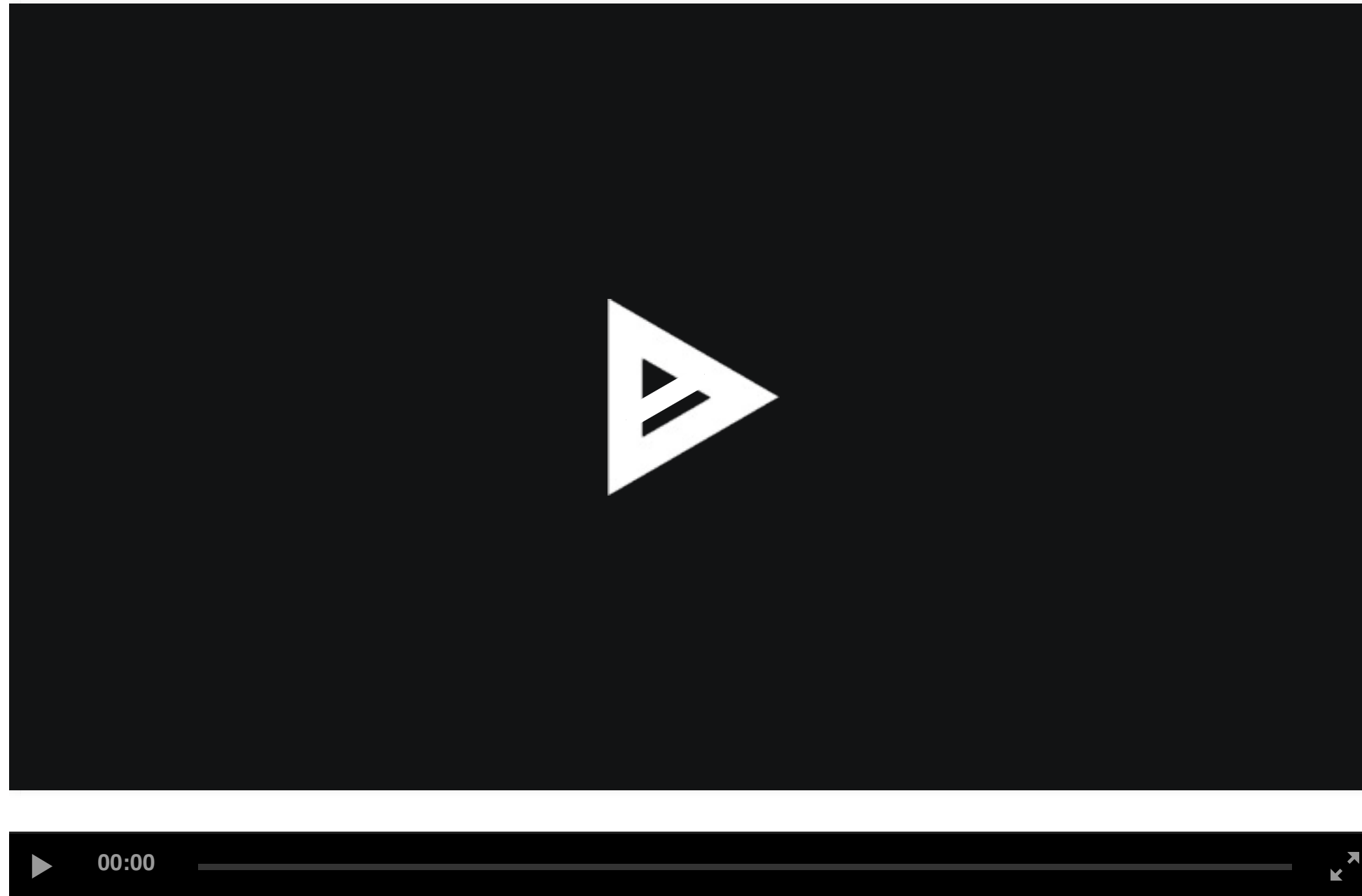
Why to **NOT** use a Virtual Cluster?

- Significant Setup / Configuration Required
- OS Administration Expertise Required
- Custom software use cases handled by Singularity

Installing Cloudmesh Client

- Create VirtualEnv for Cloudmesh Client
- Install System Dependencies
- Install Cloudmesh Client with pip

Create VirtualEnv for Cloudmesh Client



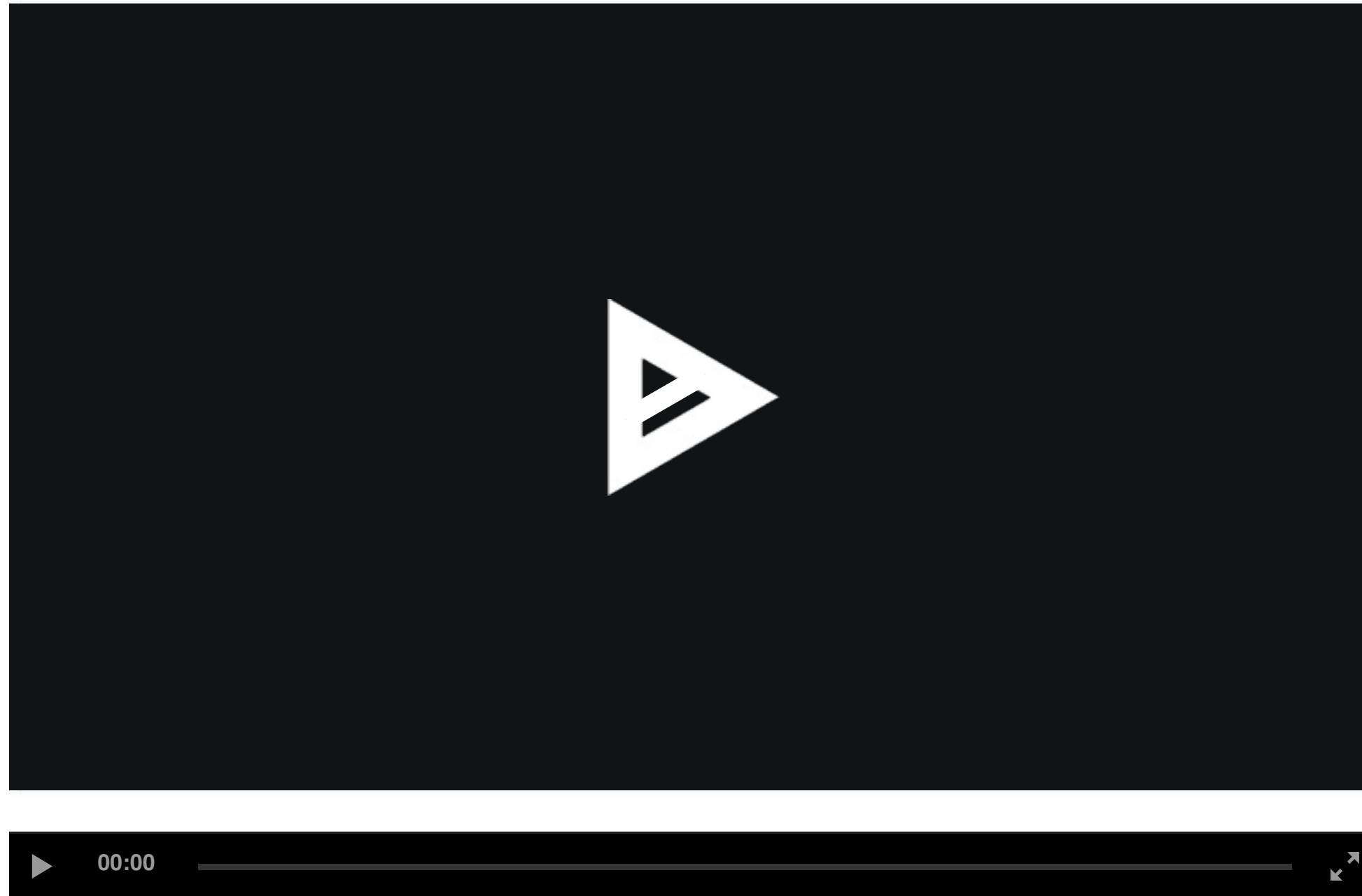
<https://asciinema.org/a/129877>

Install System Dependencies



<https://asciinema.org/a/129879>

Install Cloudmesh Client with pip

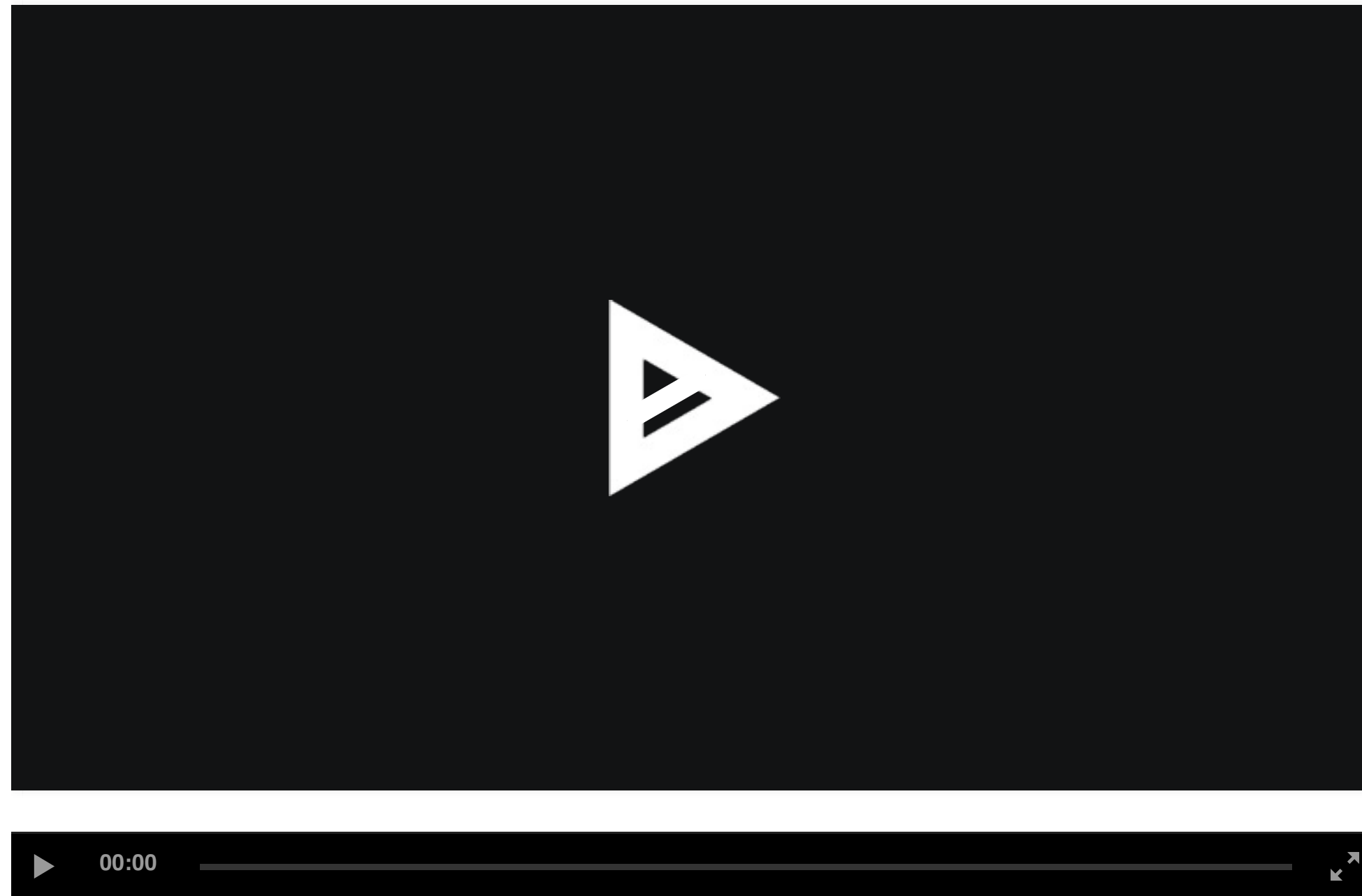


<https://asciinema.org/a/129882>

Running Cloudmesh Client

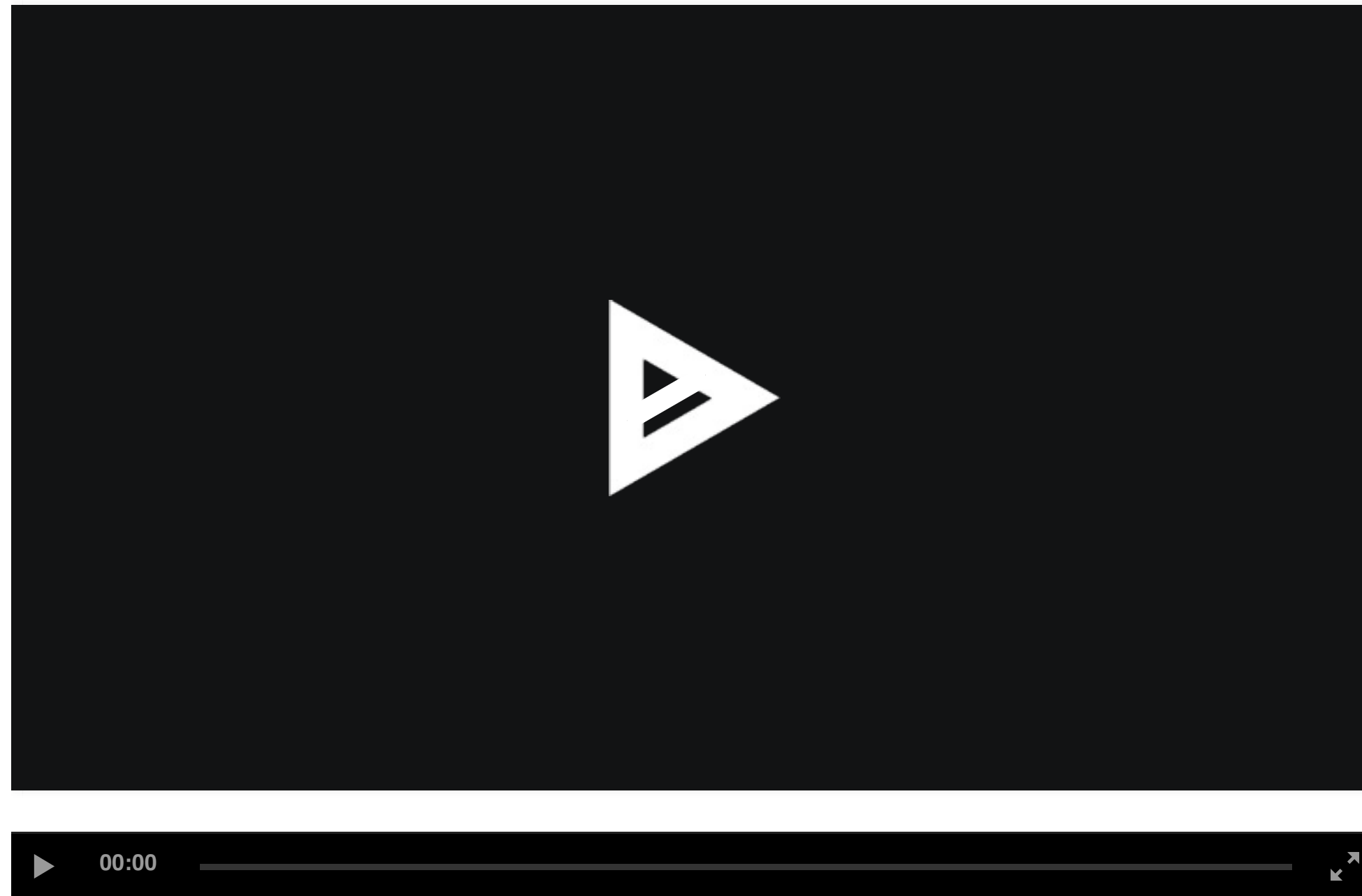
- Initialize Cloudmesh Client
- Virtual Cluster Operations

Initialize Clouddmesh Client



<https://asciinema.org/a/129883>

Virtual Cluster Operations



<https://asciinema.org/a/129885>

comet-nucleus-dev.sdsc.edu

Comet Virtual Cluster Console - vct02

Virtual Cluster Console: vct02

SDSC SAN DIEGO SUPERCOMPUTER CENTER

```
Ubuntu 16.04.2 LTS vct02 tty1
vct02 login: _
```

COMET

IS HERE

SDSC