

Singularity Containers and Comet Virtual Clusters

SDSC Summer Institute - 2017

Presented by Trevor Cooper

Overview

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

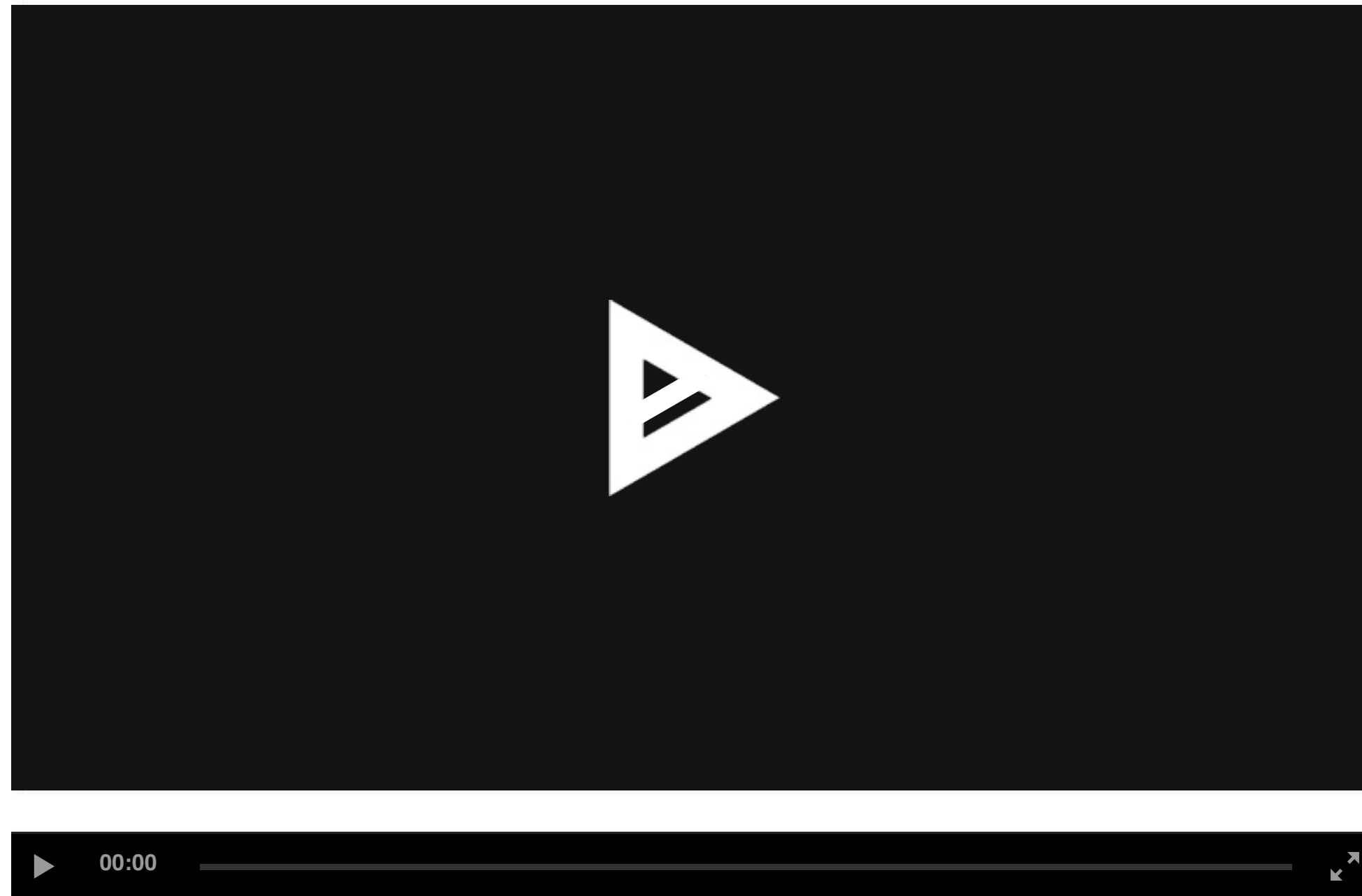
Download & Install Singularity

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

Go to the Singularity website and download...

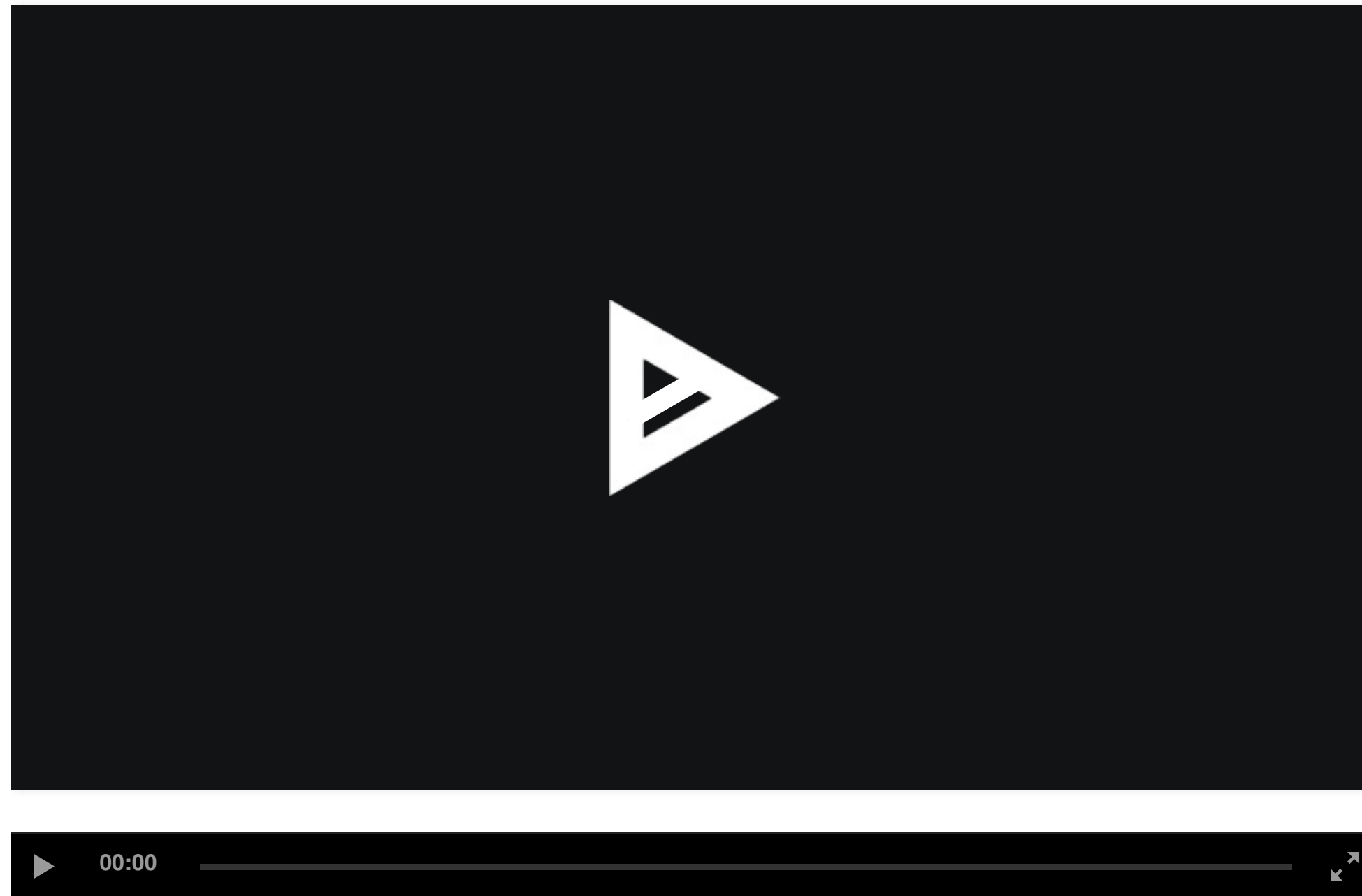
<http://singularity.lbl.gov/install-linux>

Download & Unpack Singularity



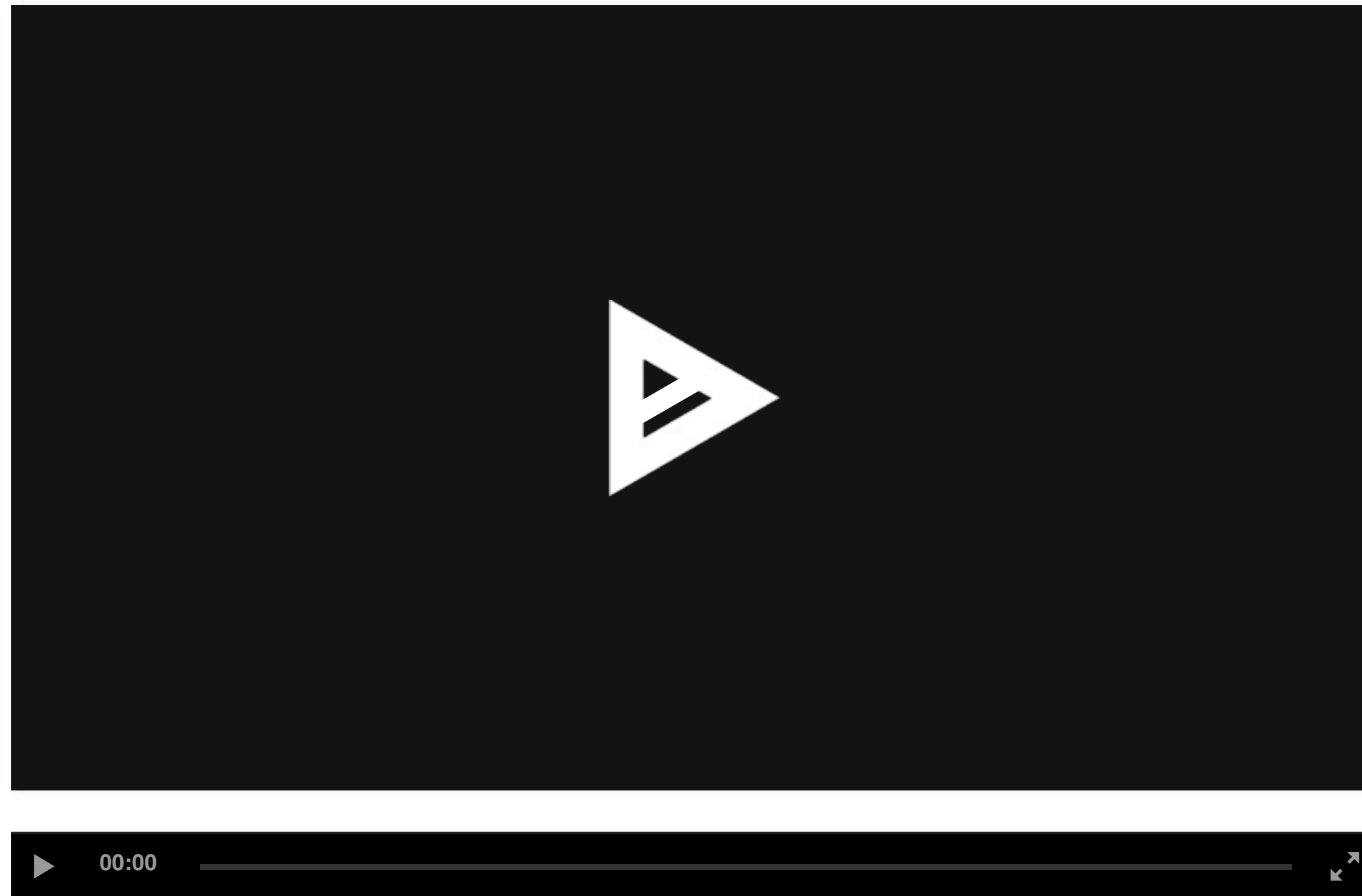
<https://asciinema.org/a/129866>

Configure & Build Singularity



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

Install & Test Singularity

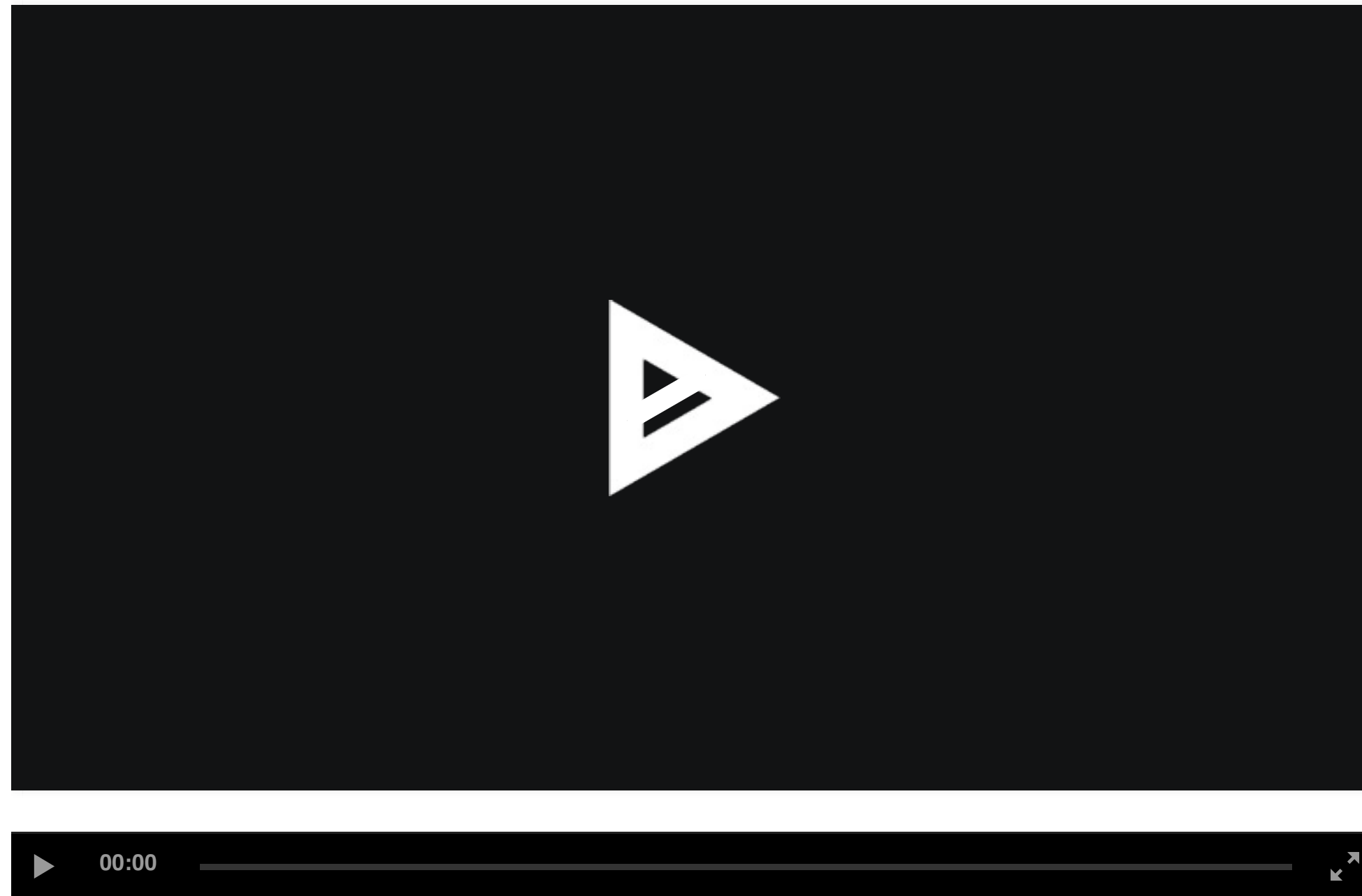


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Building Singularity Containers

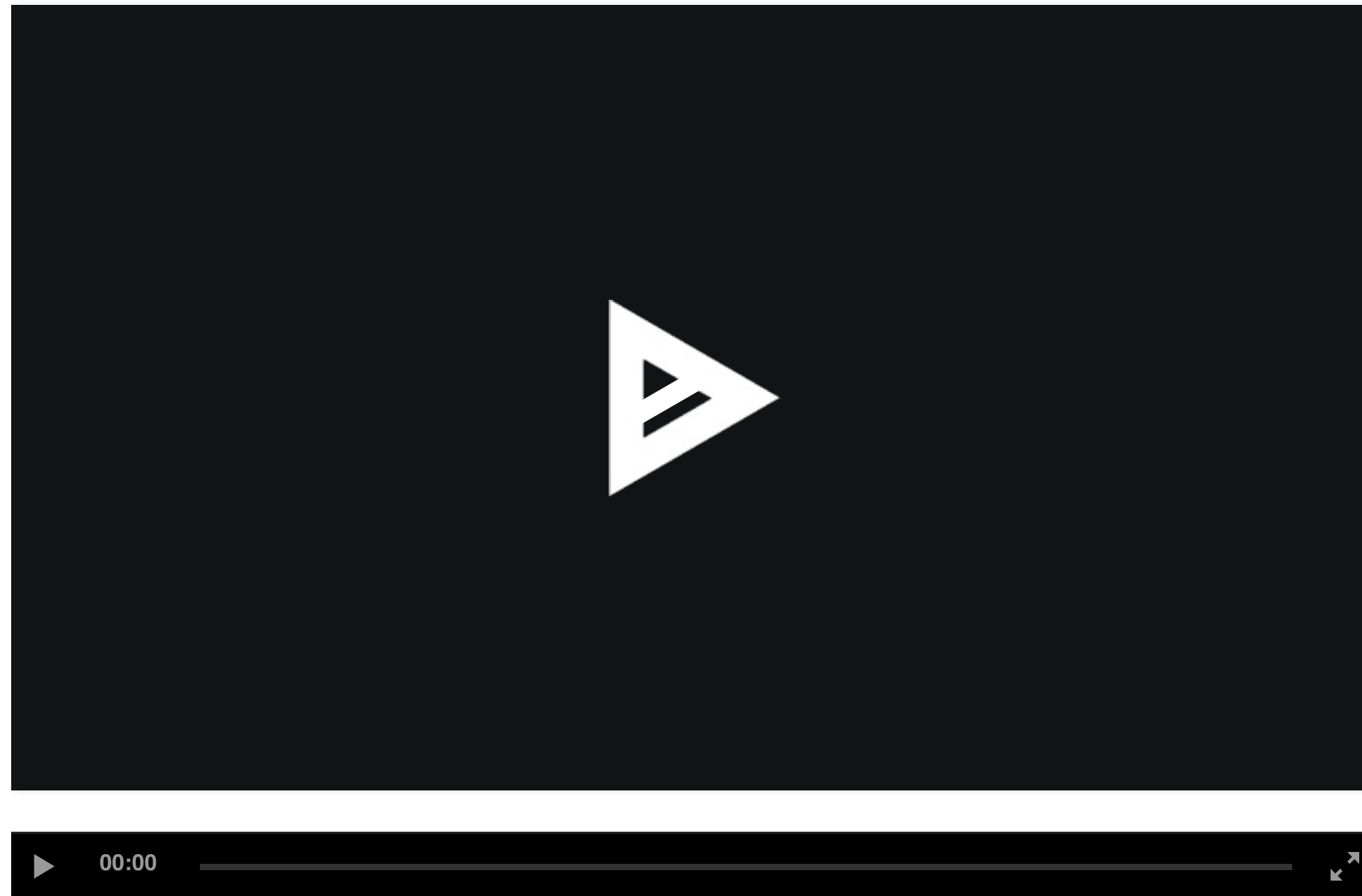
- Create Empty Container
- Import into Container
- Shell into Container
- Write into Container
- Bootstrap Container

Create Empty Container



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

Import Into Container



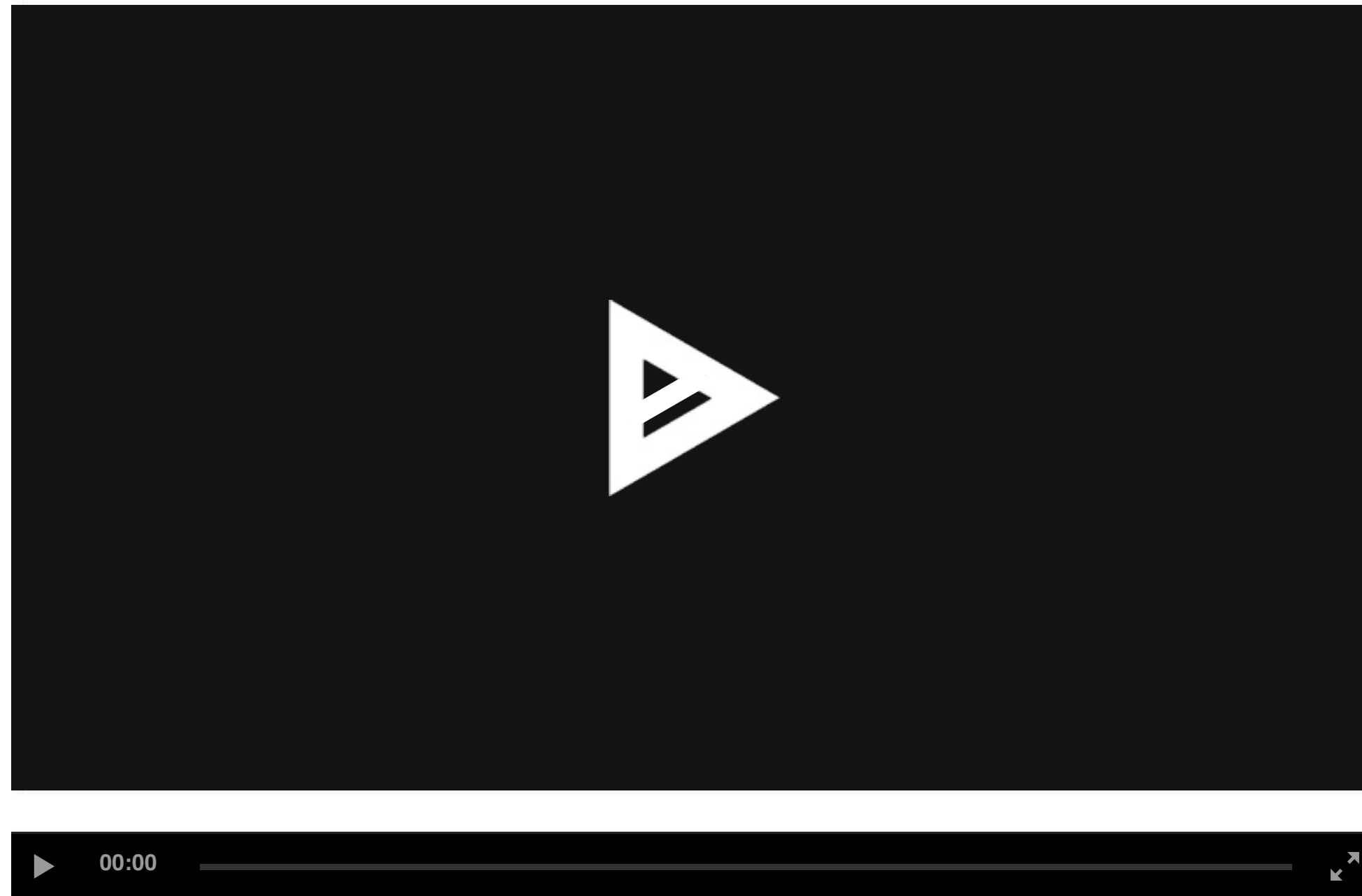
<https://asciinema.org/a/130107>

Shell into Container



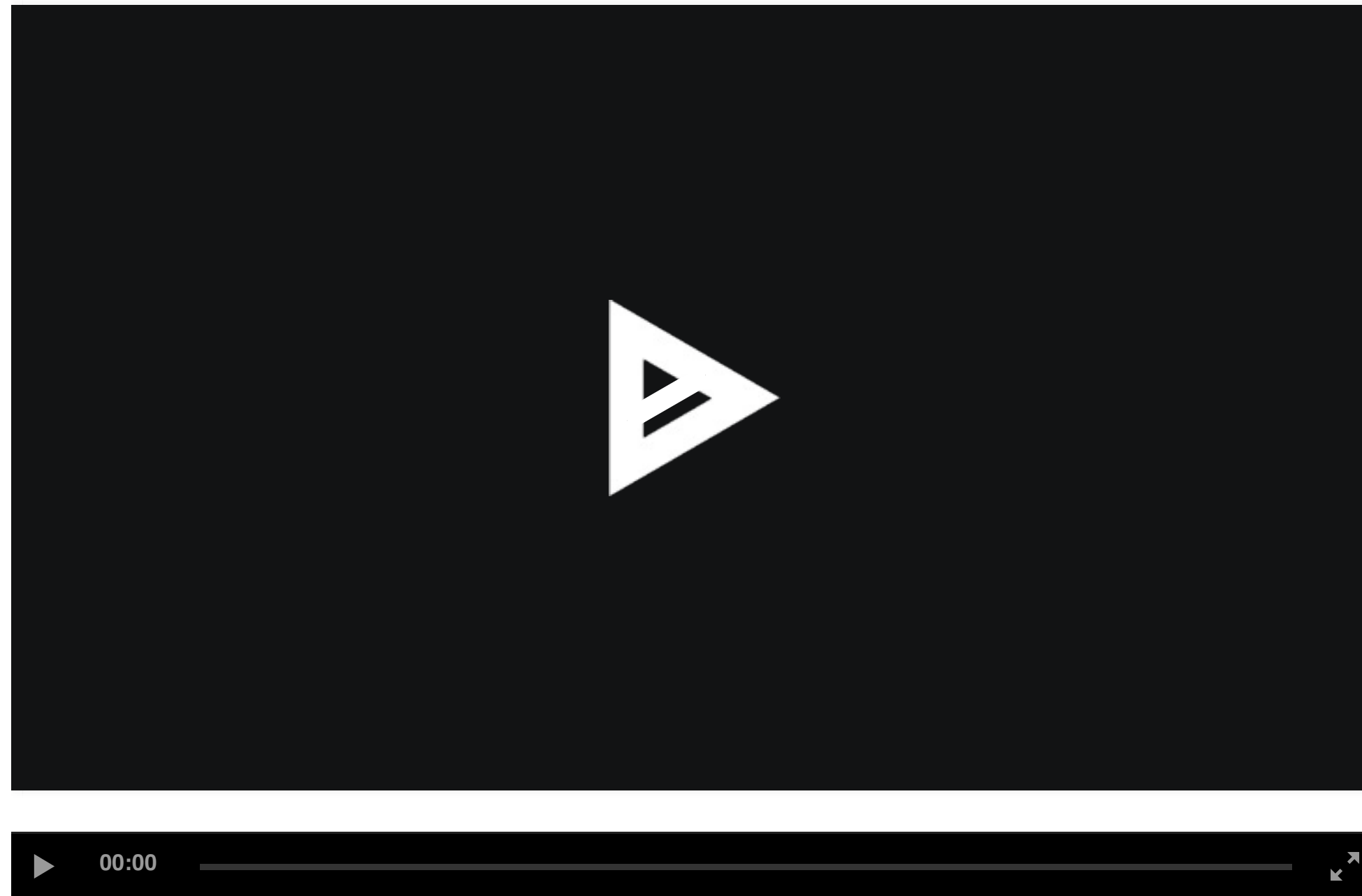
<https://asciinema.org/a/130109>

Write into Singularity Container



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

Bootstrap Container



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

Running Singularity Containers on Comet

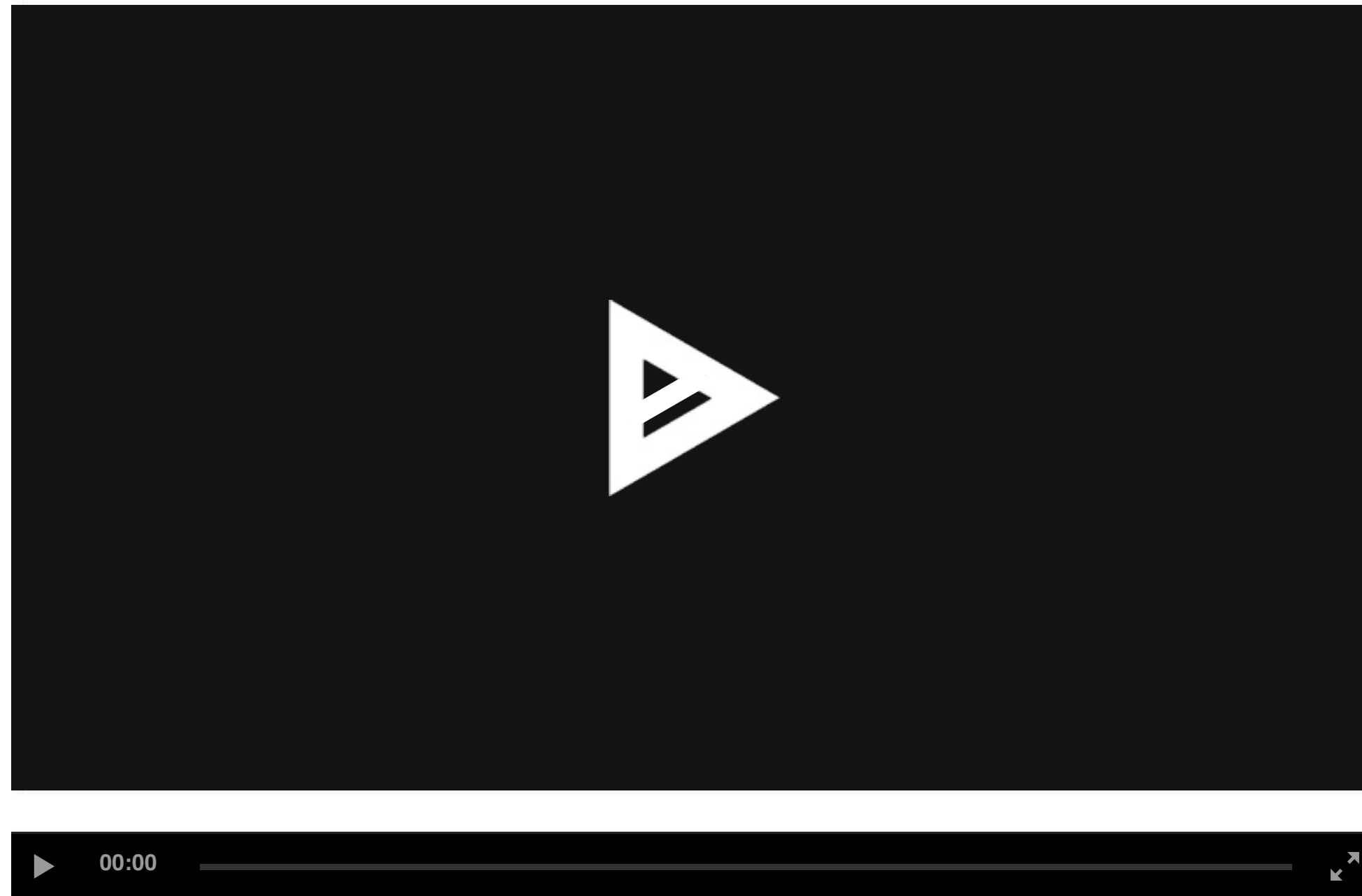
- Transfer Container to Comet
- Run Container on Comet
- Allocate Resources to Run Container
- Integrate Container with Slurm

Transfer Container to Comet



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

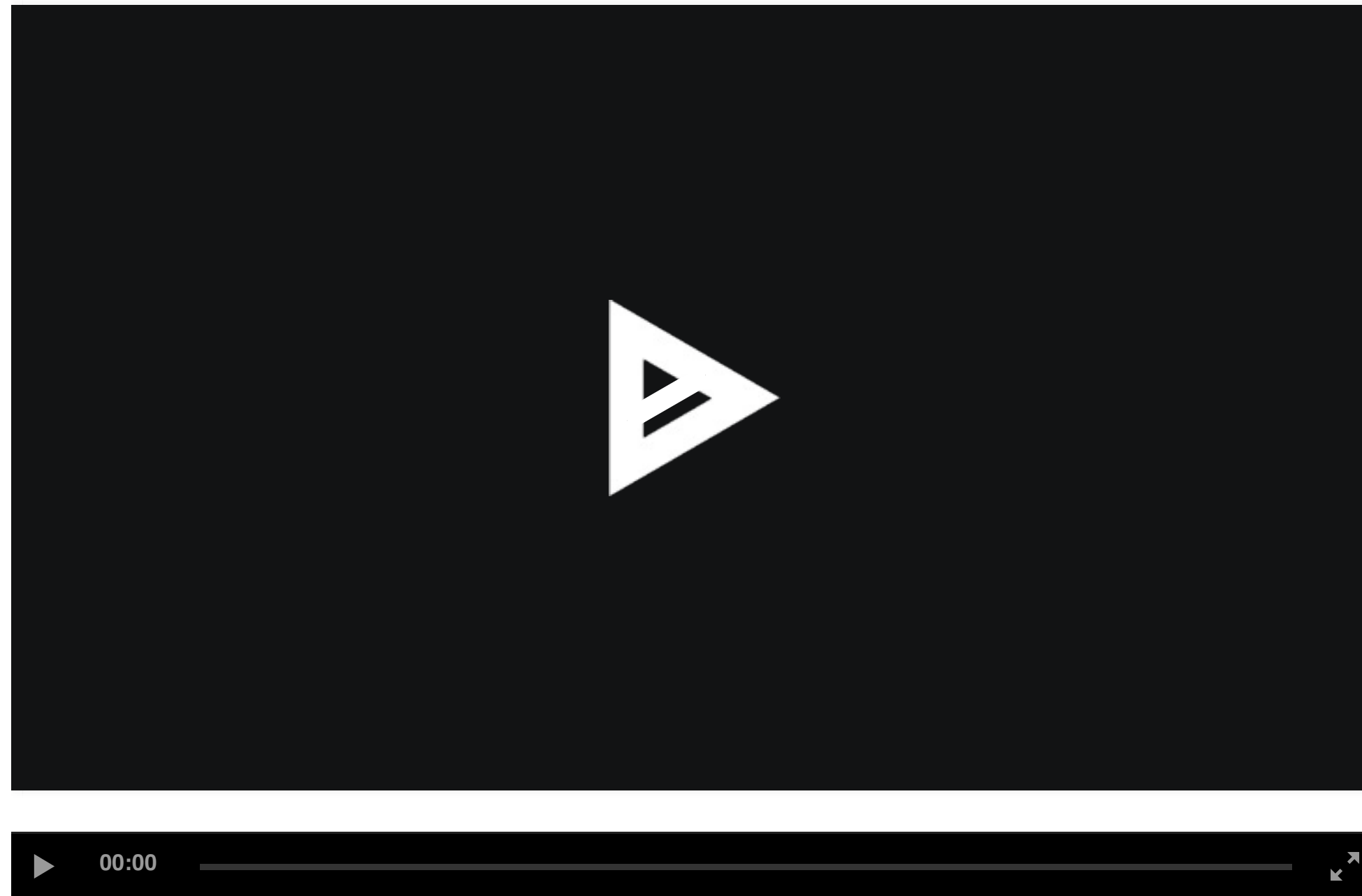
Run Container on Comet



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

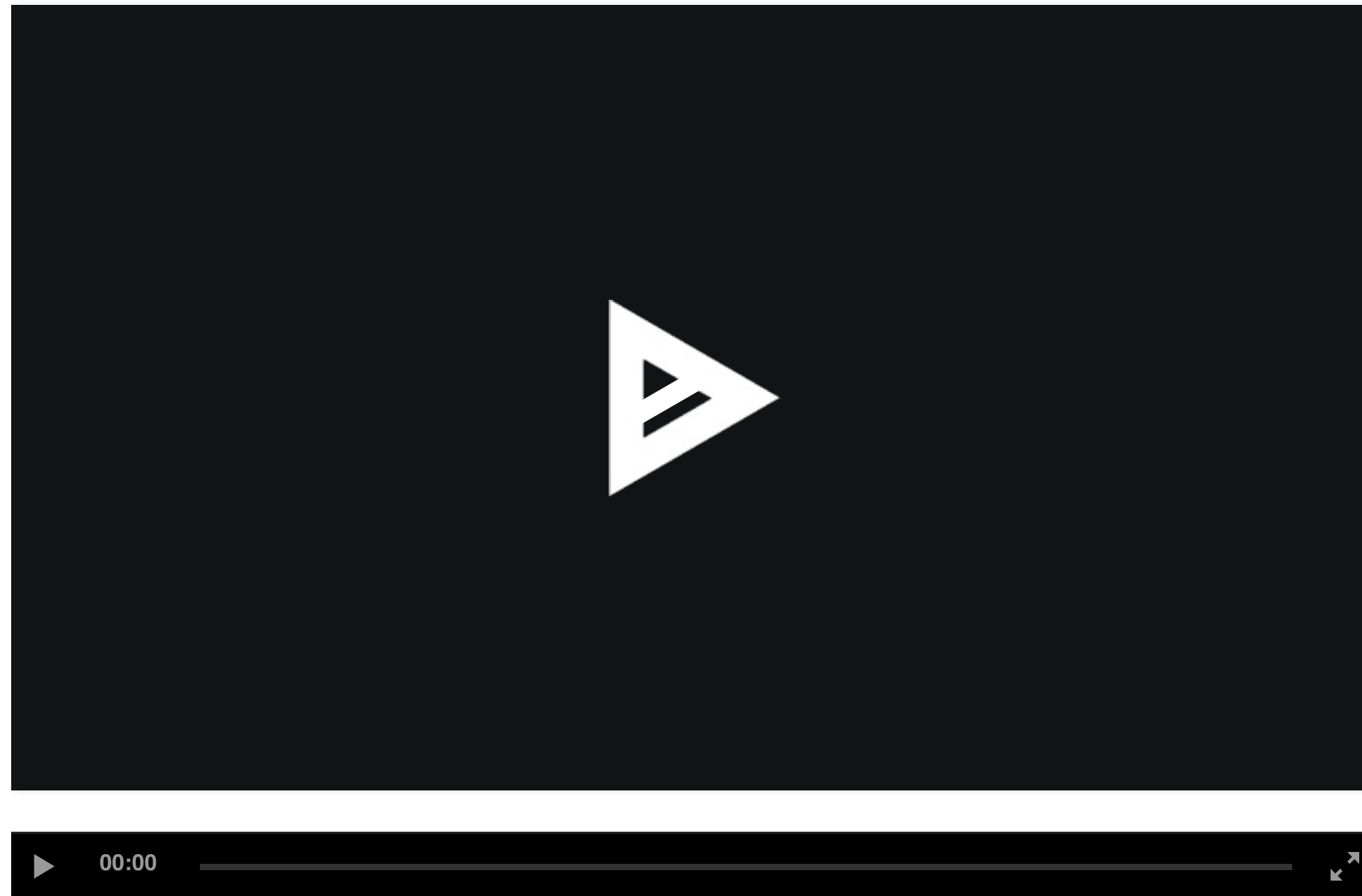
Allocate Resources to Run Container

17



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

Integrate Container with Slurm

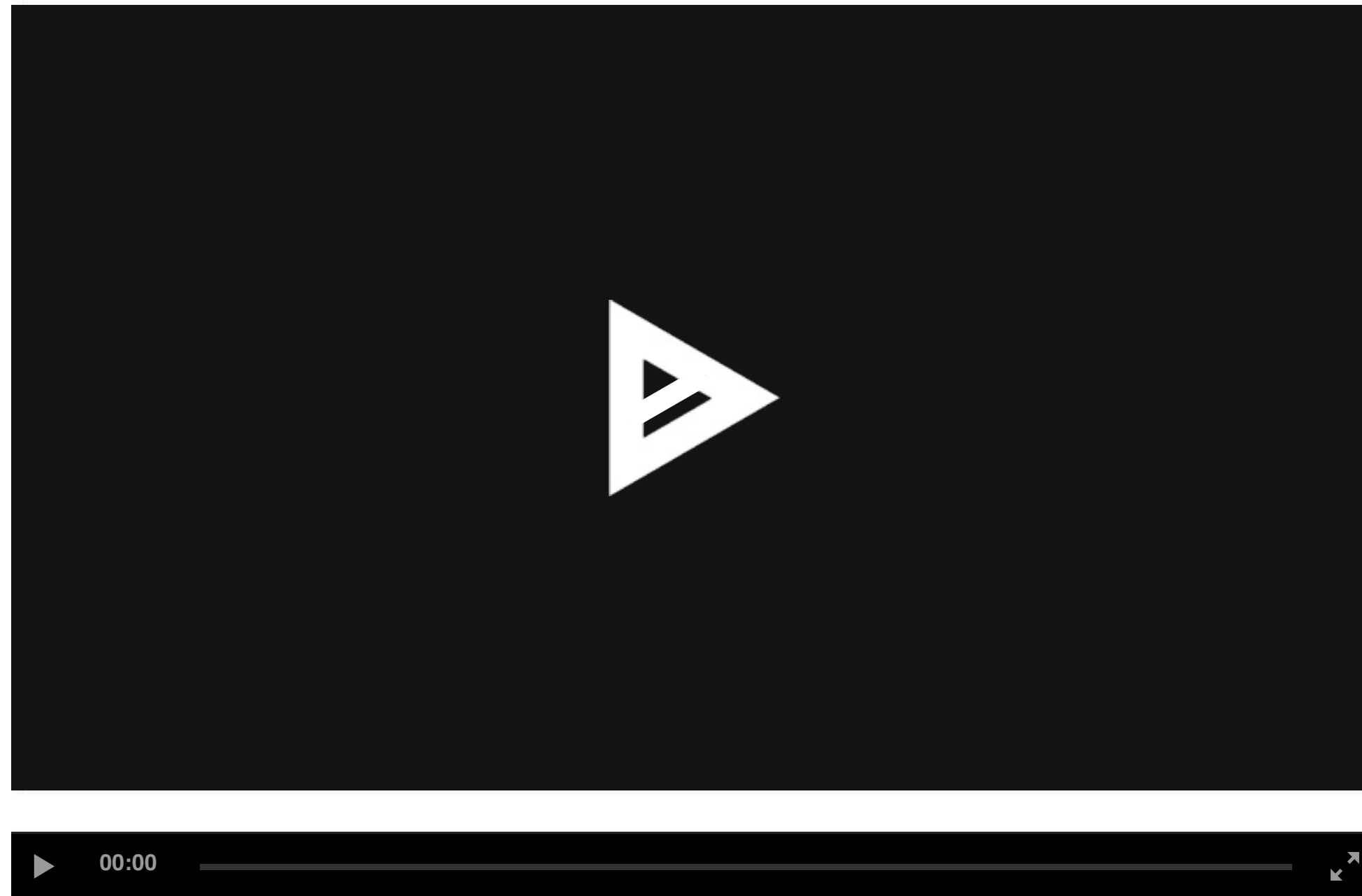


<https://asciinema.org/a/130218>

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 URL. The GitHub navigation bar at the top includes the repository name, a search bar, and links for Pull requests, Issues, Marketplace, and Gist. The repository header shows the name `hpcdevops / singularity-hello-world` and statistics: 0 Watchers, 0 Stars, and 0 Forks. Below the header, there are tabs for Code, Pull requests (0), Projects (0), and Insights. The main content area features the repository description "Simple hello world container for Singularity" and a summary bar with 9 commits, 2 branches, 0 releases, and 1 contributor. A row of buttons includes "Branch: master", "New pull request", "Create new file", "Upload files", "Find file", and "Clone or download". The commit history table lists four commits: the latest commit `e5adfc2` by `hpcdevops` updating the README (17 hours ago), and three previous commits for `LICENSE`, `README.md`, and `Singularity` (all 2 days ago).

hpcdevops/singularity-hello-world: Simple hello world container for Singularity

This repository Search Pull requests Issues Marketplace Gist

hpcdevops / singularity-hello-world Watch 0 Star 0 Fork 0

Code Pull requests 0 Projects 0 Insights

Simple hello world container for Singularity

9 commits 2 branches 0 releases 1 contributor

Branch: master New pull request Create new file Upload files Find file Clone or download

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...

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hpcdevops

hpcdevops/singularity-hello-world

DISCUSSIONMAKE PRIVATEBRANCHESEDIT BUILDERSHARE

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...

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hpcdevops

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

Score: 0.6

runusrtmplliblocal-scratchetcvarsharesharenotebooks

shareliblocallib

Files

libbfd-2.24-system.solibgirepository-1.0.so.1.0.0libopcodes-2.24-system.solibperl.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

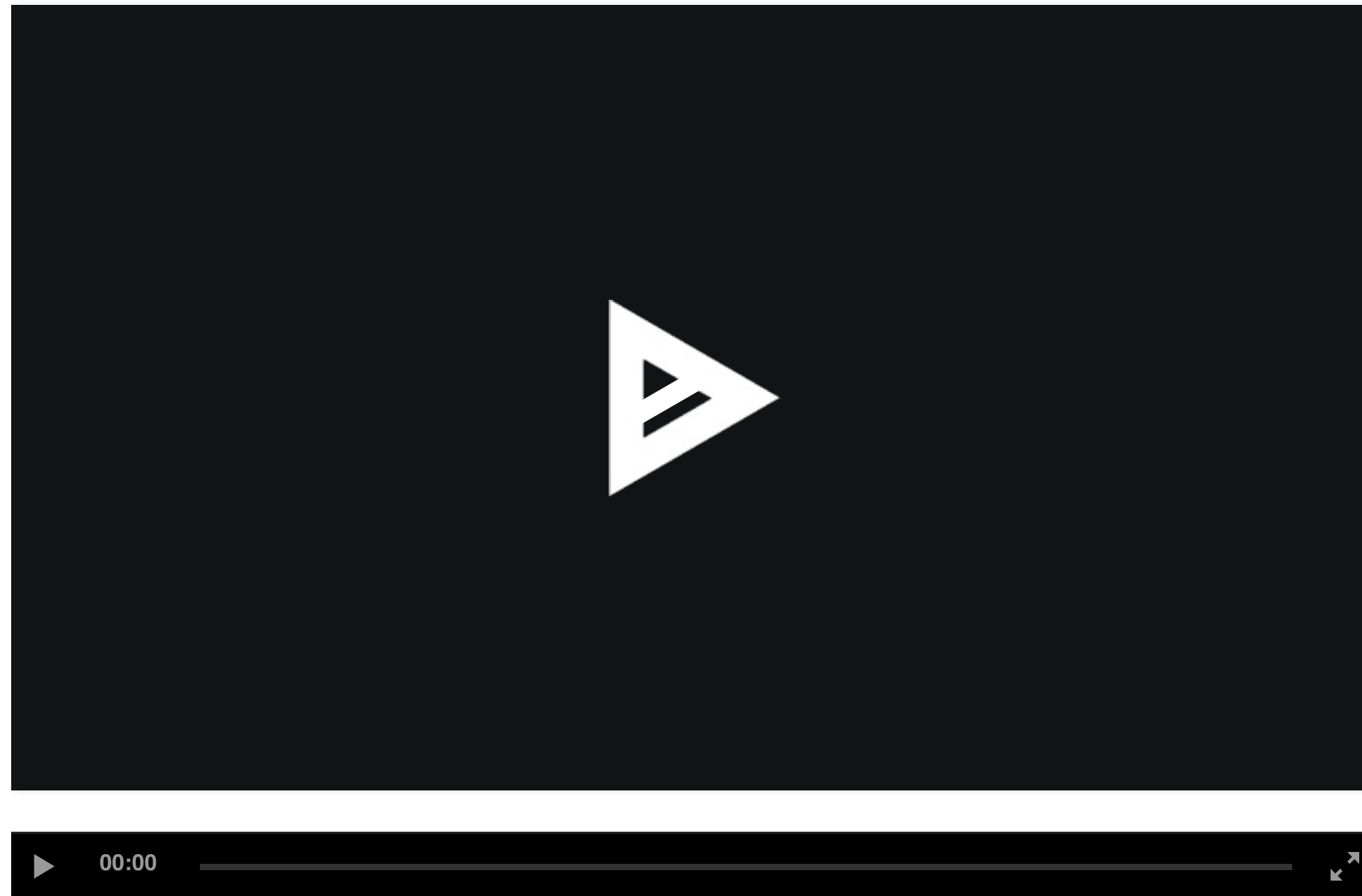
Why to **NOT** use a Virtual Cluster?

- 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



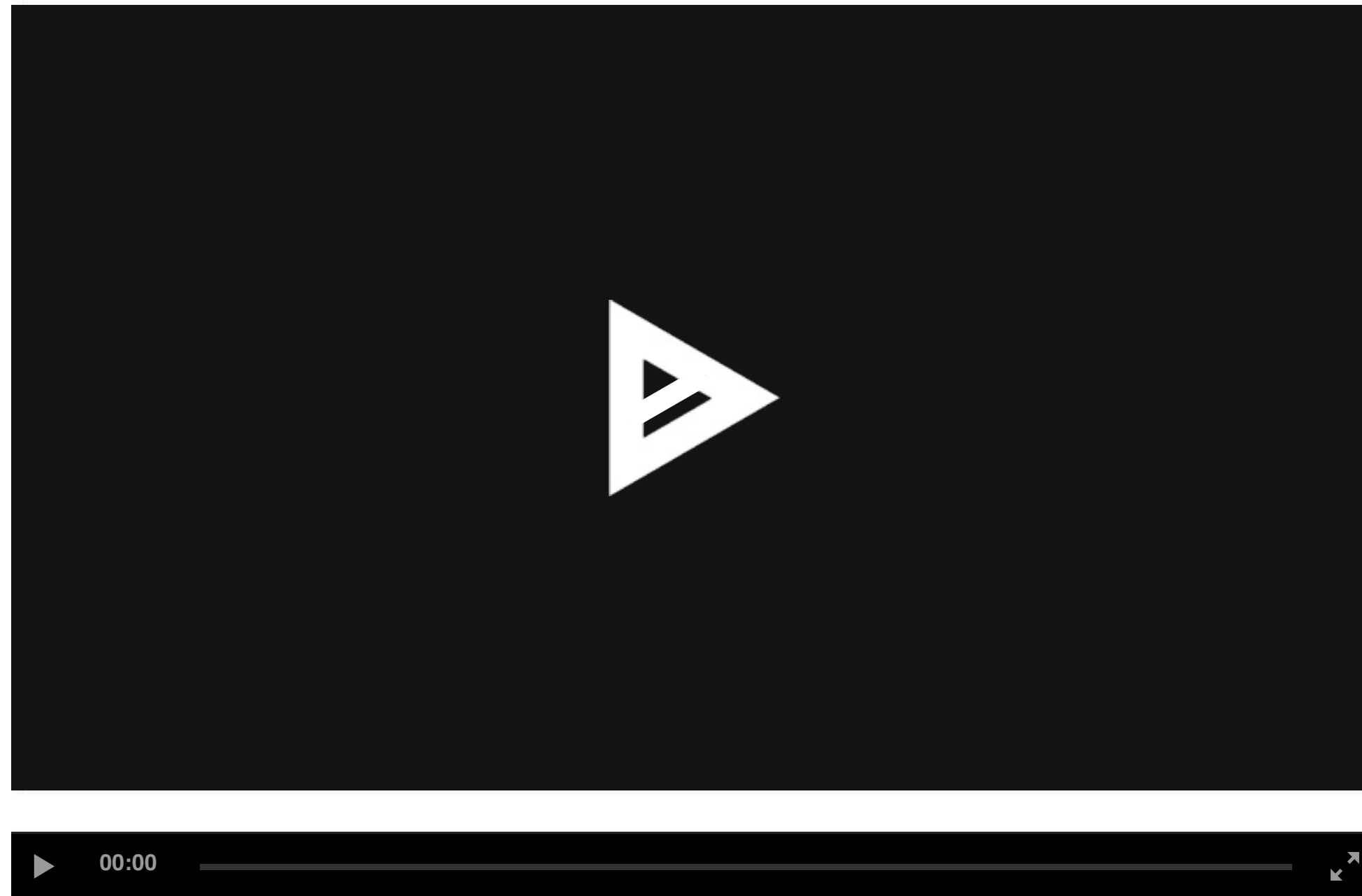
<https://asciinema.org/a/129877>

Install System Dependencies



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

Install Cloudmesh Client with pip

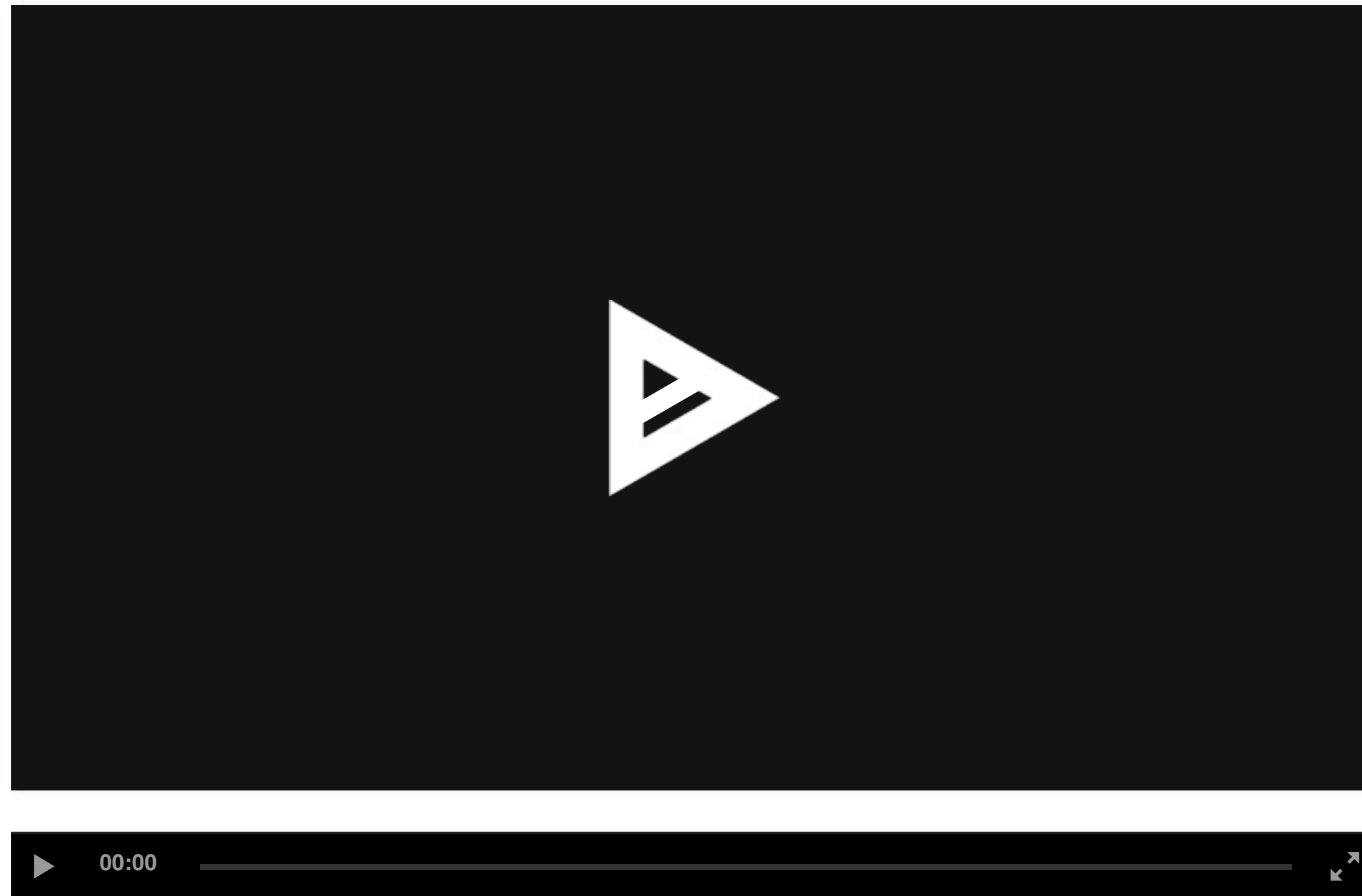


<https://asciinema.org/a/129882>

Running Cloudmesh Client

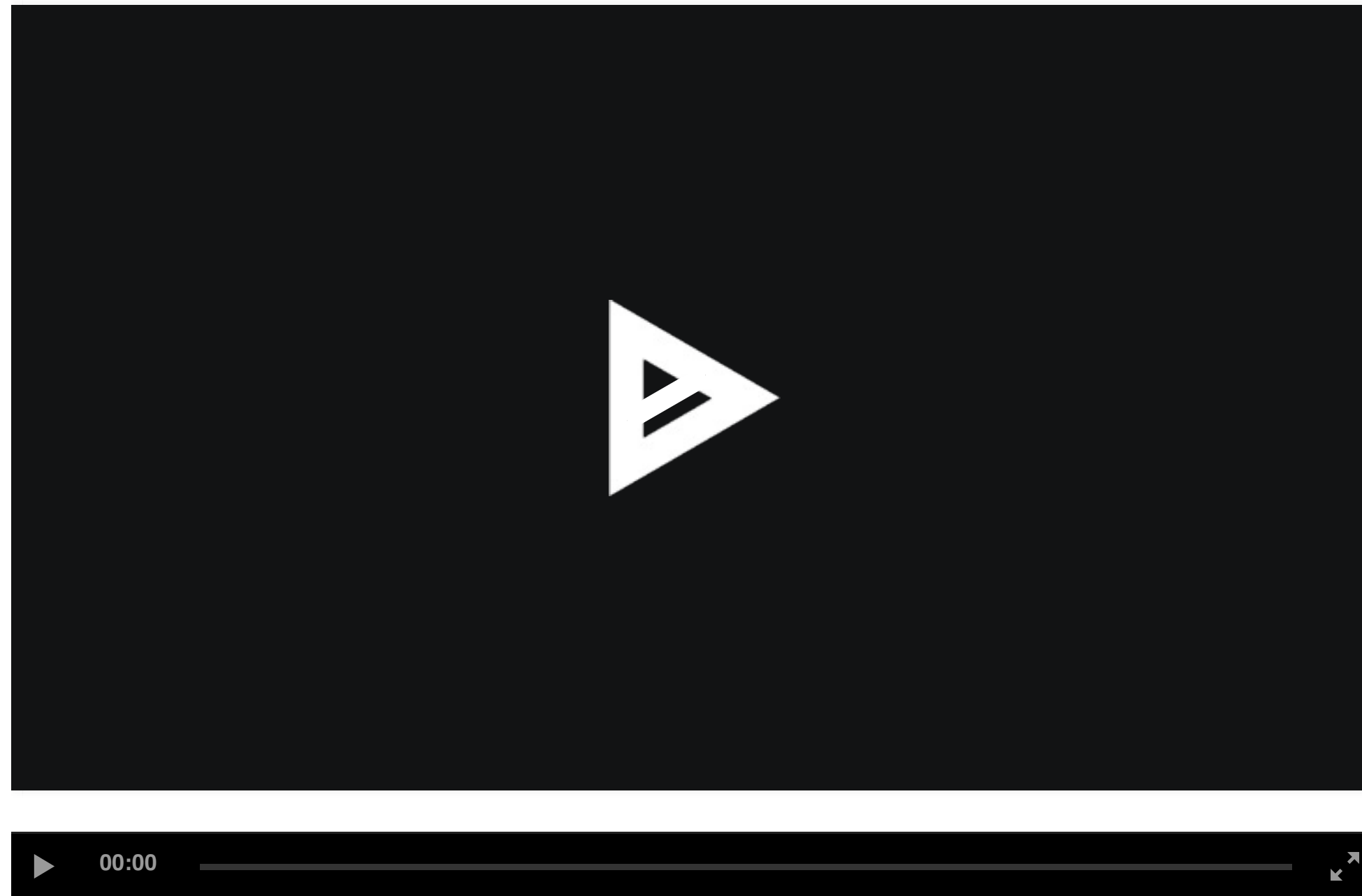
- Initialize Cloudmesh Client
- Virtual Cluster Operations

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

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