

A photograph of the San Diego Supercomputer Center at night. The building is a modern, multi-story structure with large glass windows and concrete pillars. The interior lights are on, and the building is illuminated by streetlights. The sky is dark blue.

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

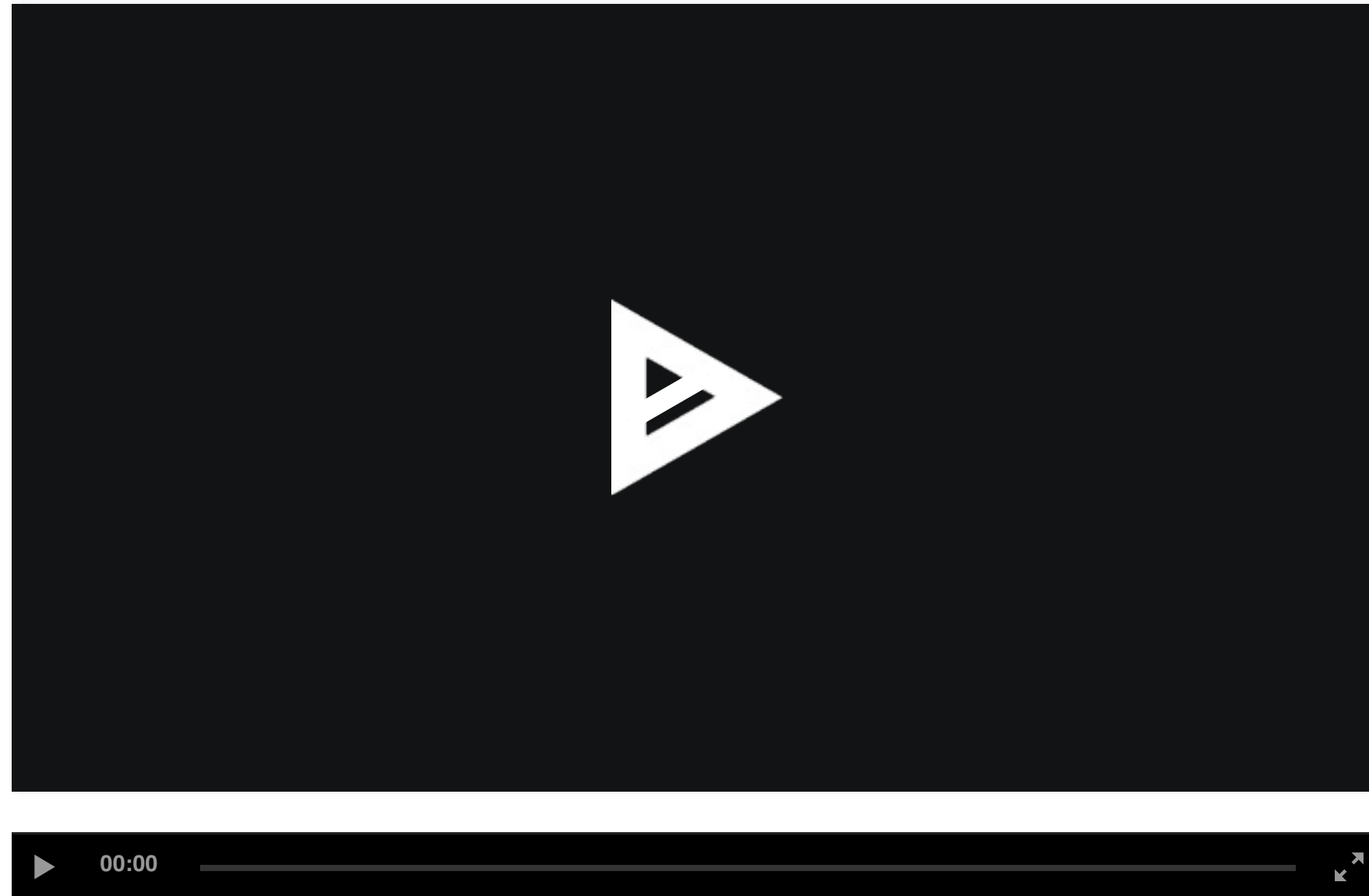
Download & Install Singularity

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

Go to the Singularity website and download...

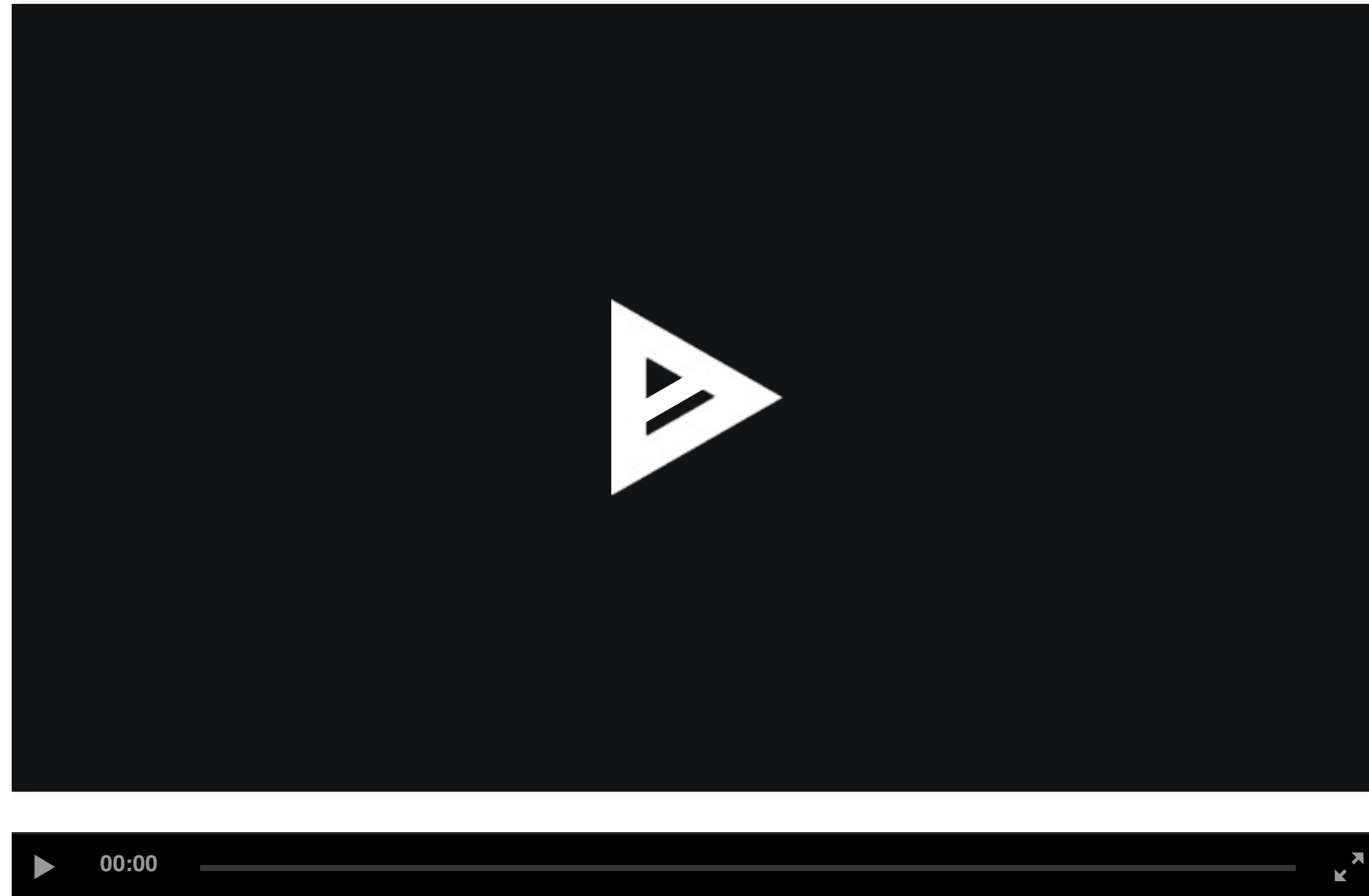
<http://singularity.lbl.gov/install-linux>

Download & Unpack Singularity



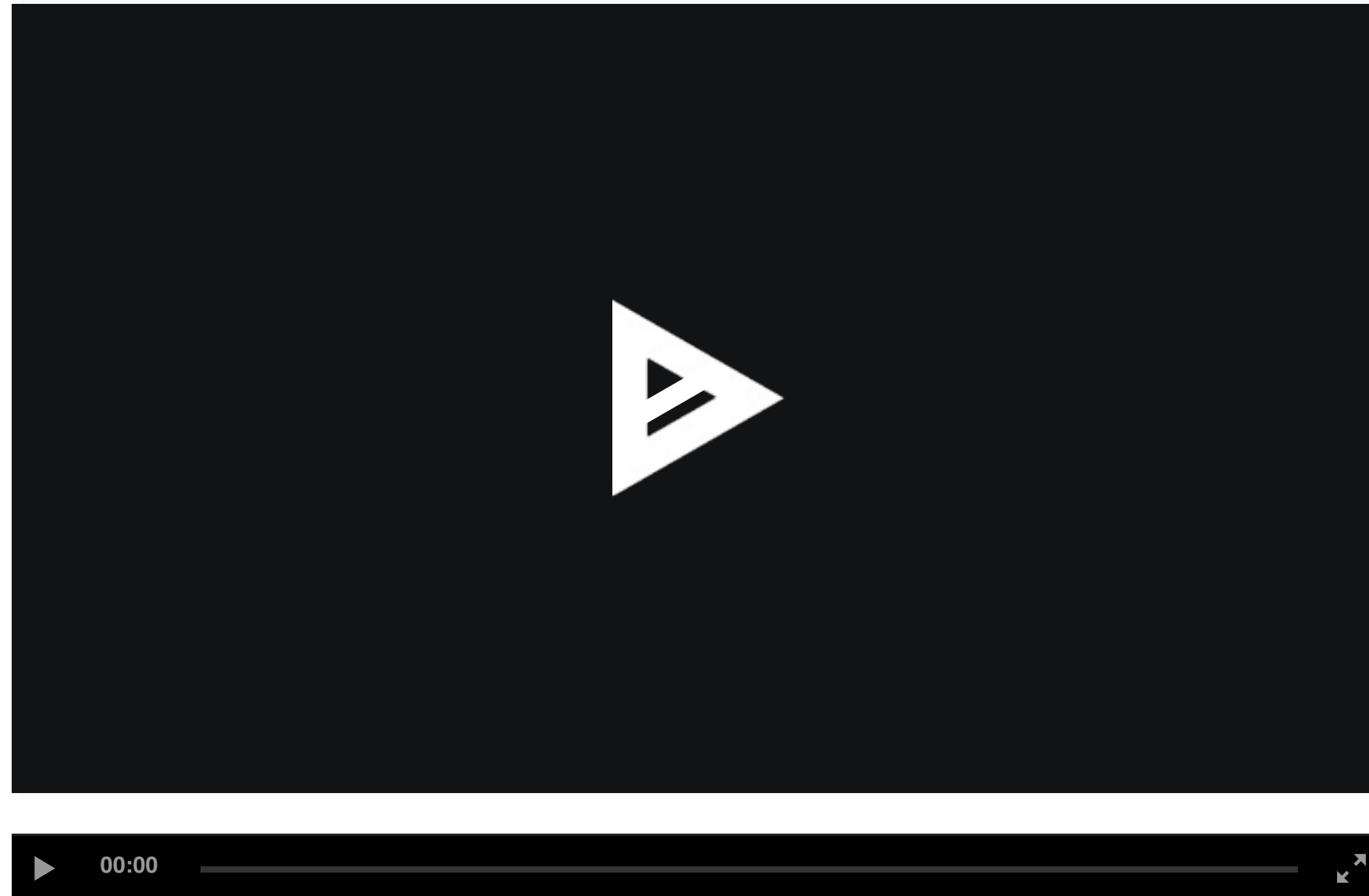
<https://asciinema.org/a/129866>

Configure & Build Singularity



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

Install & Test Singularity



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

Building Singularity Containers

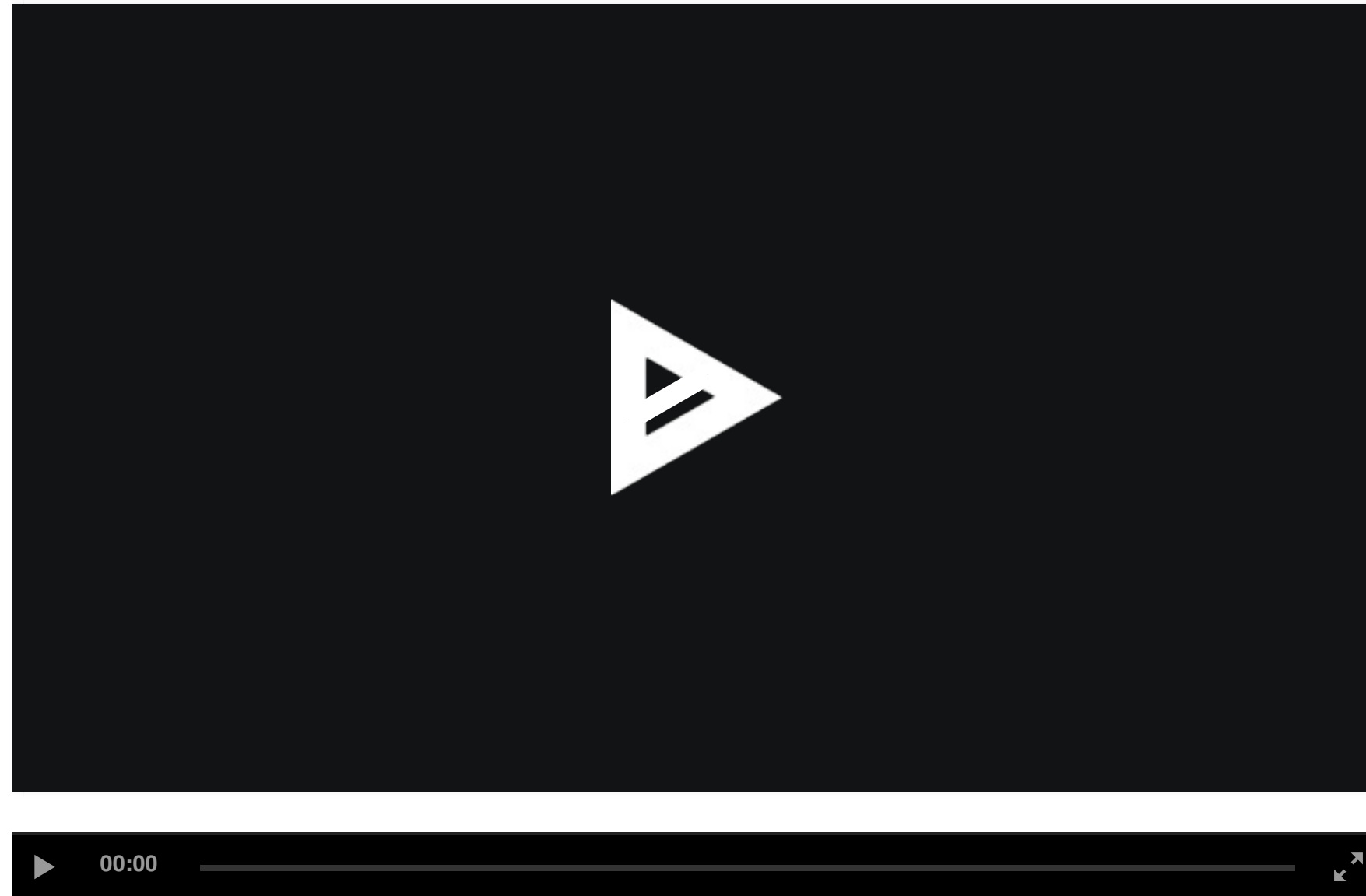
- Create Empty Container
- Import into Container
- Shell into Container
- Write into Container
- Bootstrap Container

Create Empty Container



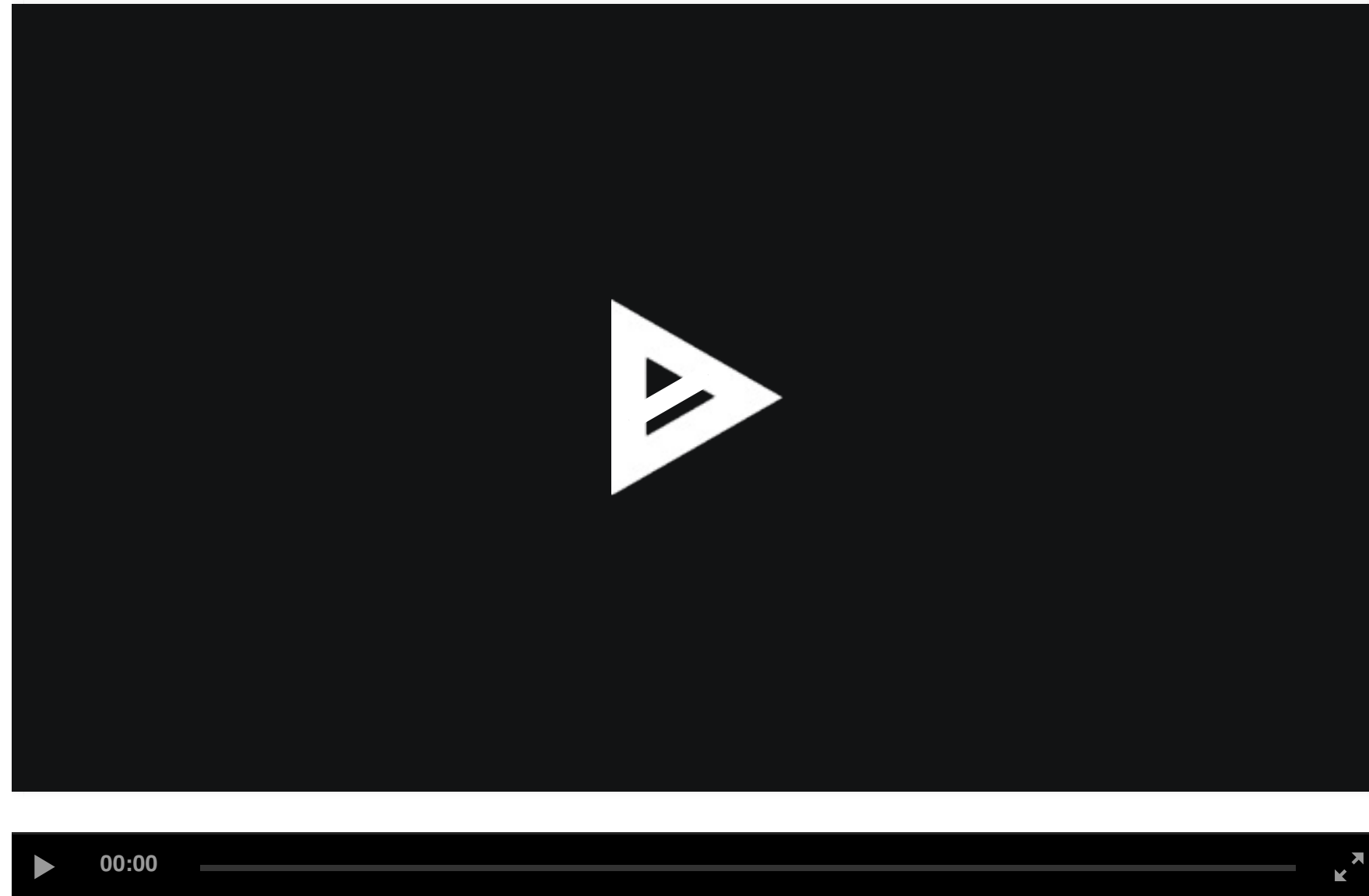
<https://asciinema.org/a/130106>

Import Into Container



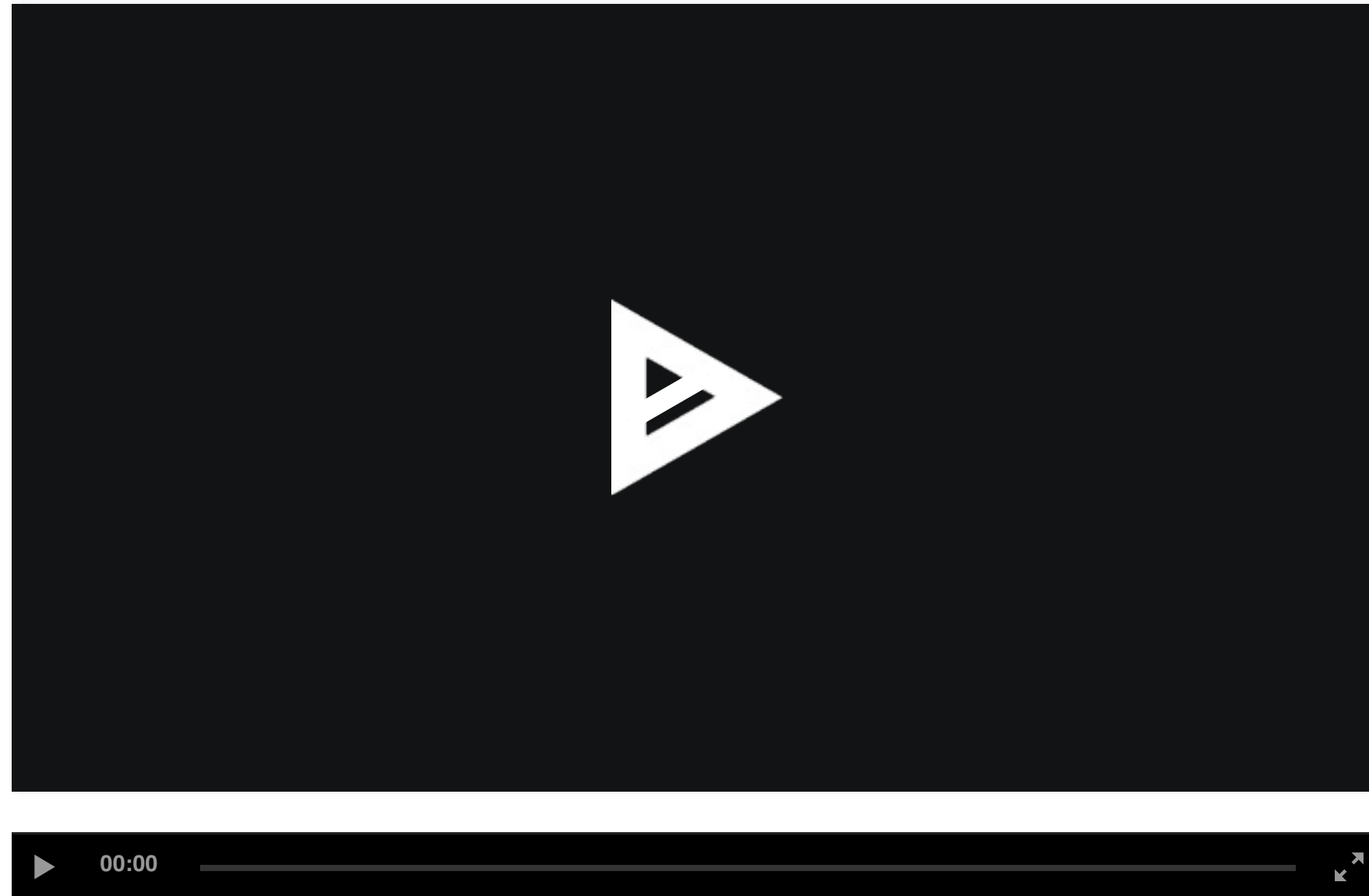
<https://asciinema.org/a/130107>

Shell into Container



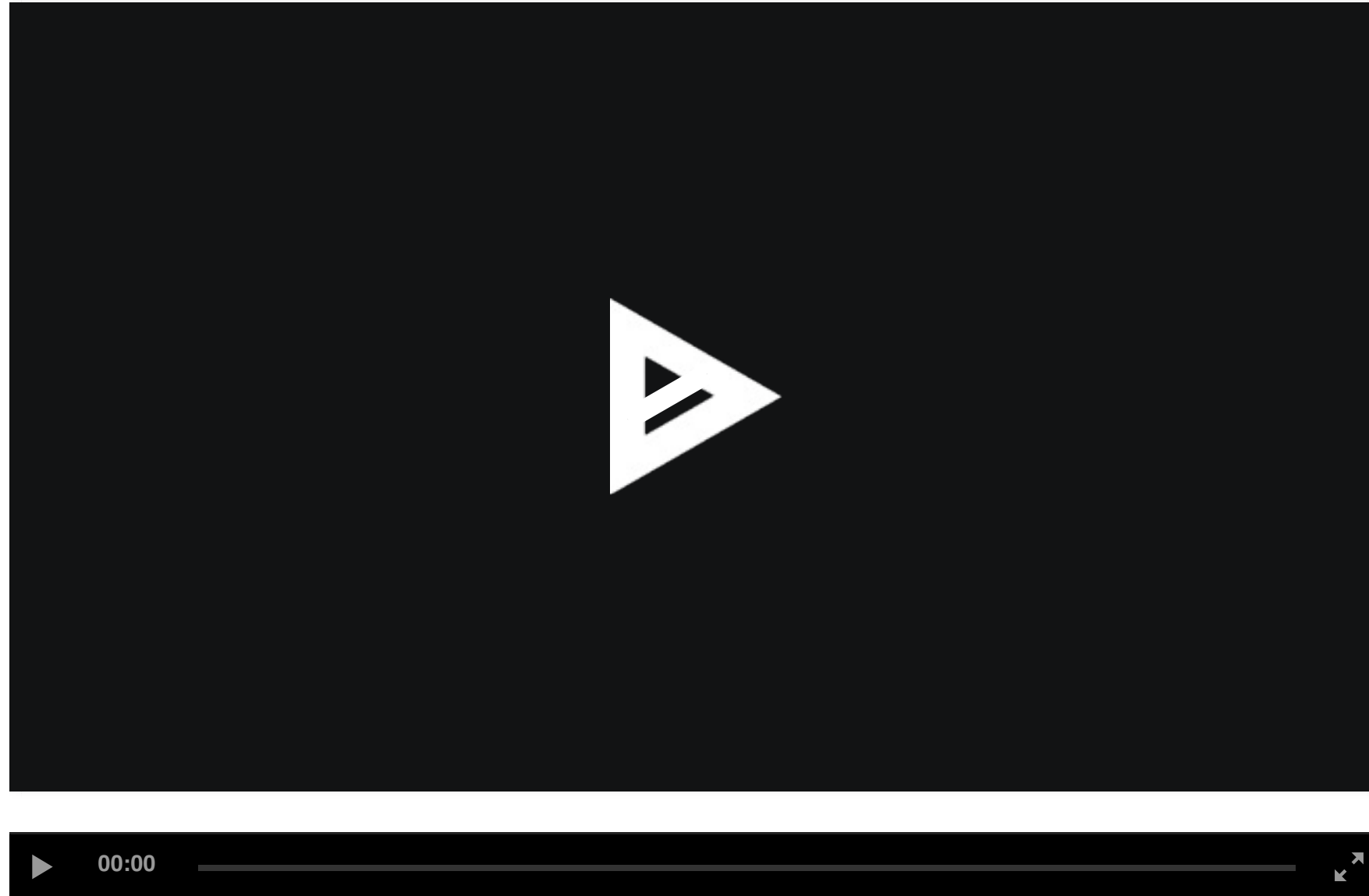
<https://asciinema.org/a/130109>

Write into Singularity Container



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

Bootstrap Container

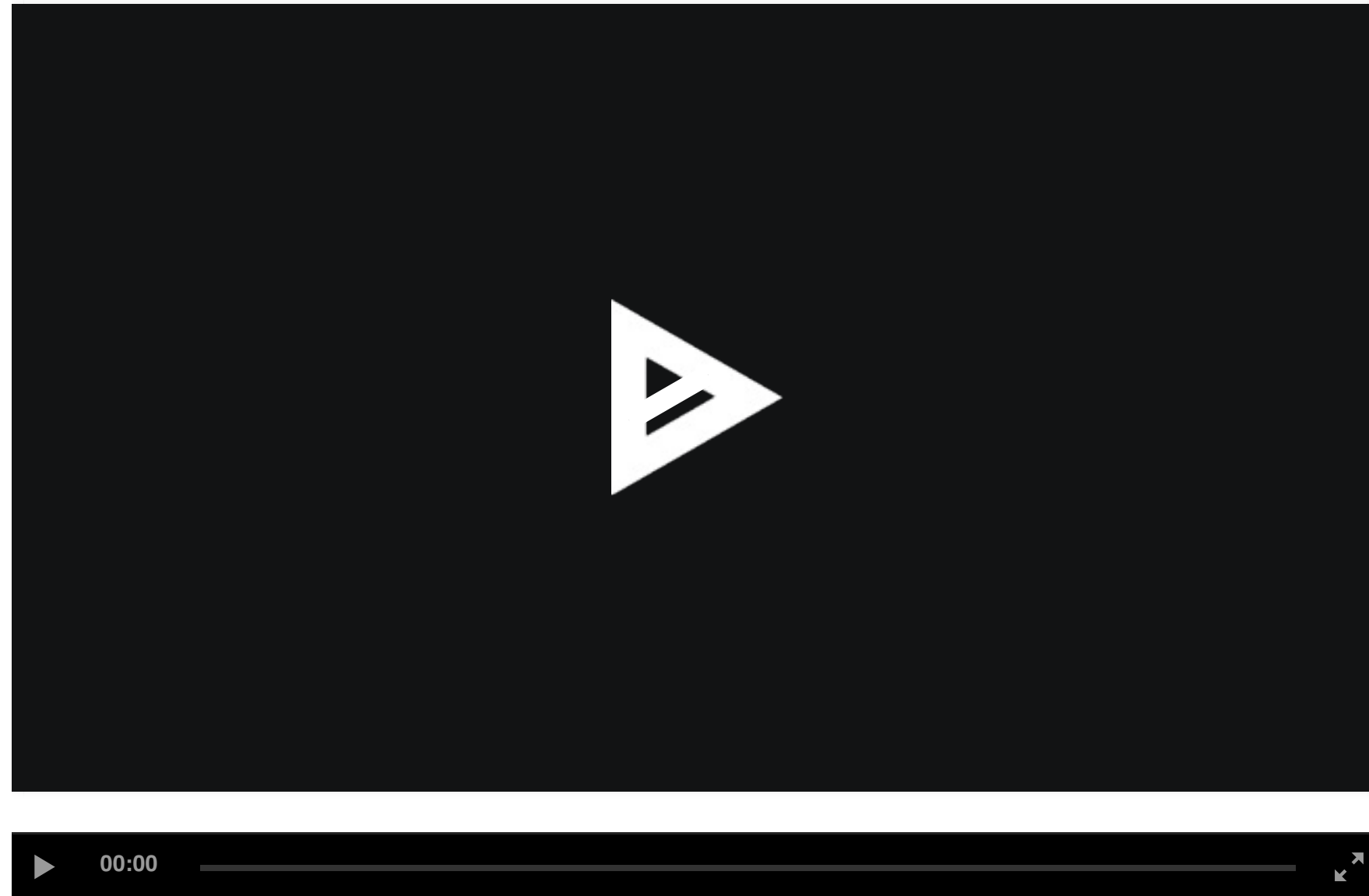


<https://asciinema.org/a/130111>

Running Singularity Containers on Comet

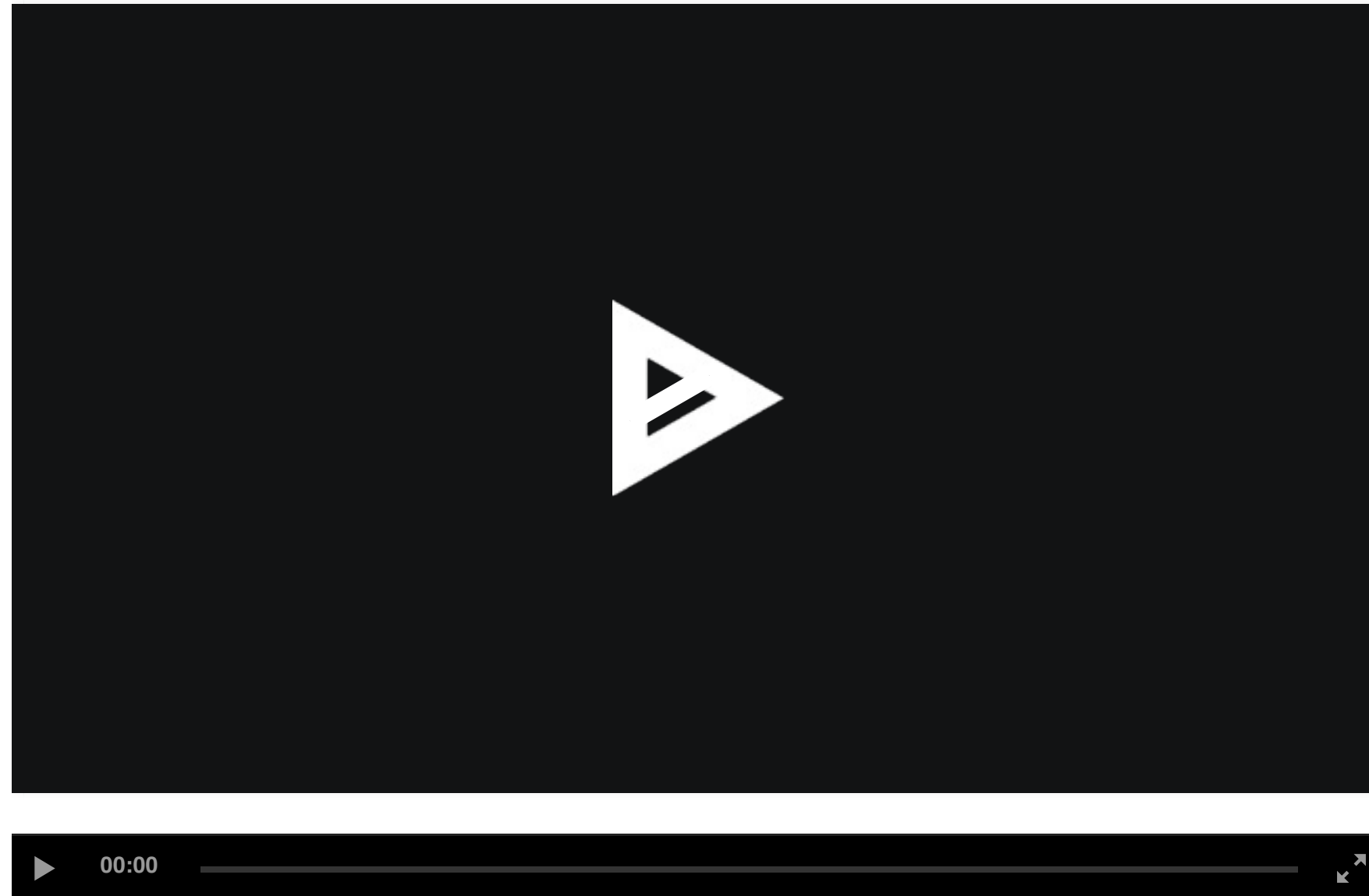
- Transfer Container to Comet
- Run Container on Comet
- Allocate Resources to Run Container
- Integrate Container with Slurm

Transfer Container to Comet



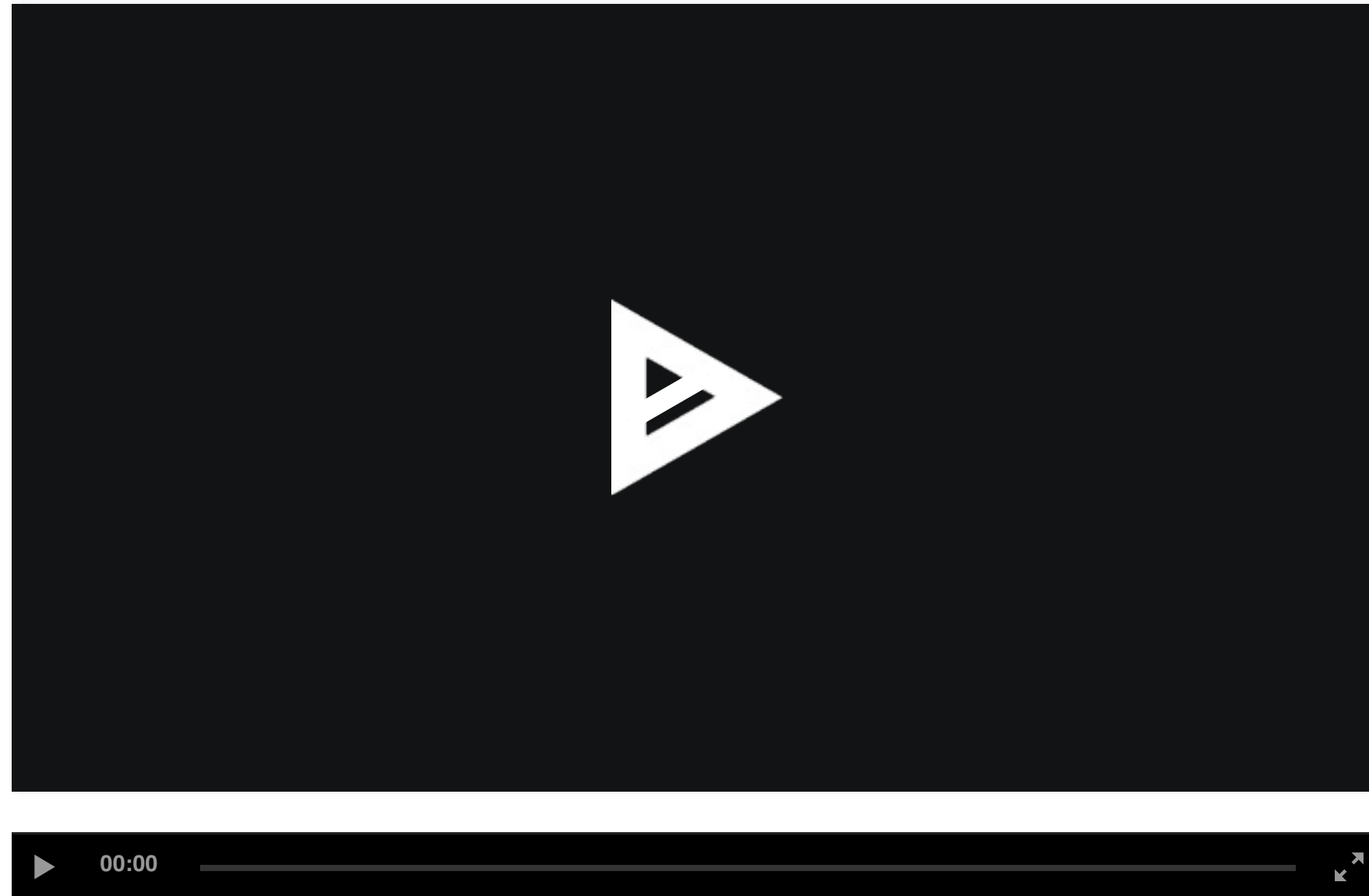
<https://asciinema.org/a/130195>

Run Container on Comet



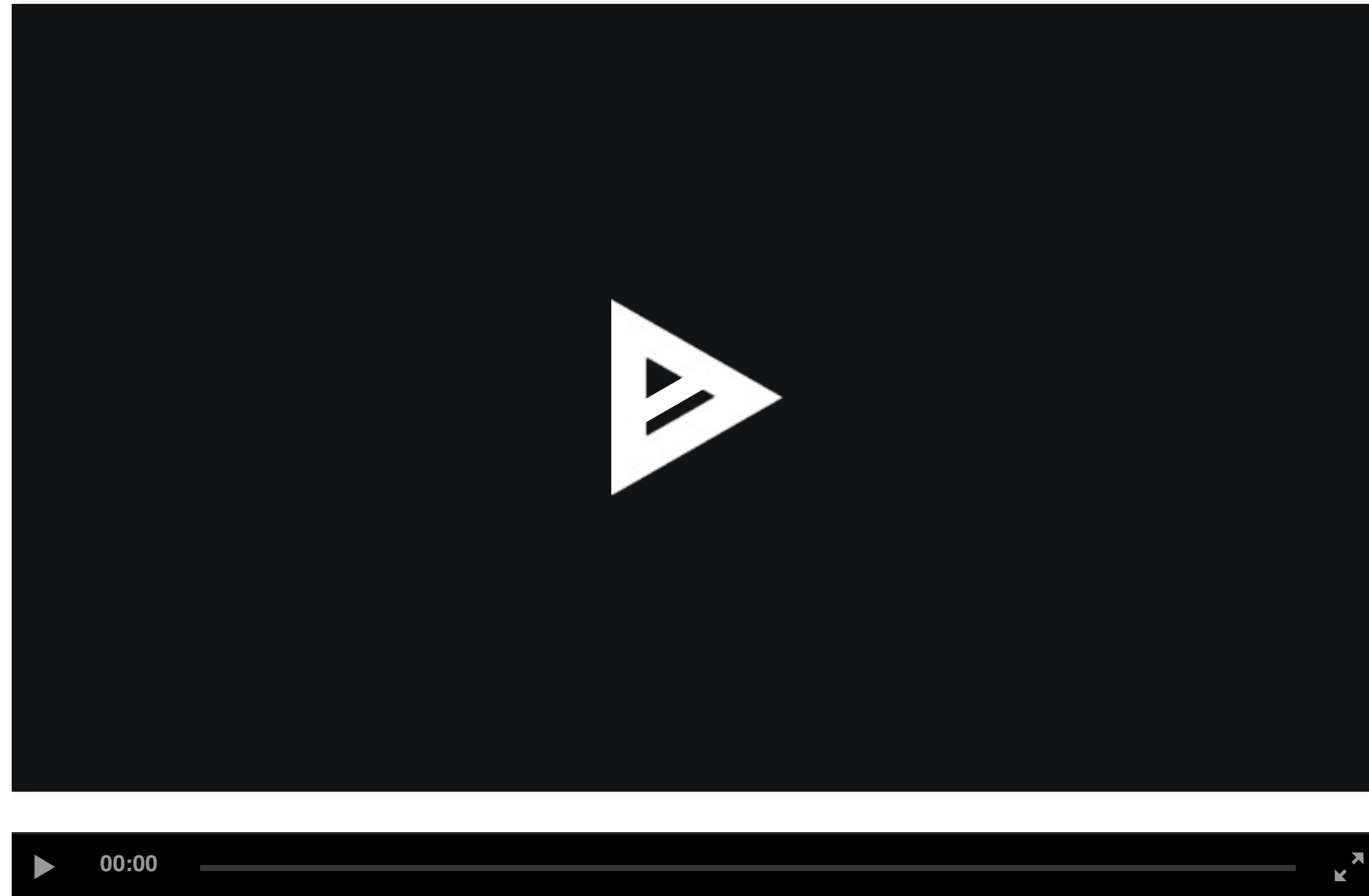
<https://asciinema.org/a/130196>

Allocate Resources to Run Container



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

Integrate Container with Slurm

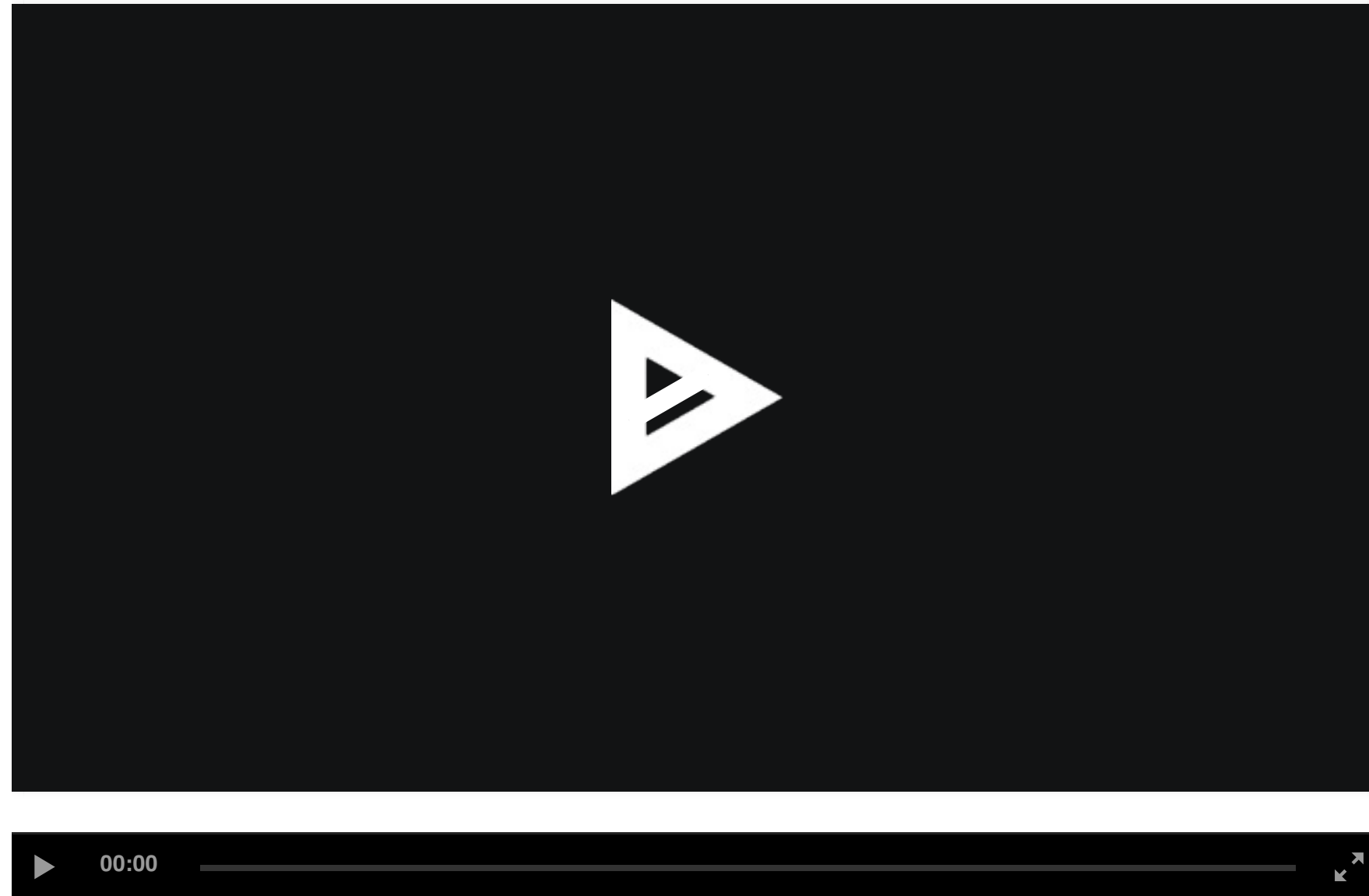


<https://asciinema.org/a/130218>

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...

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


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
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...









SINGULARITYContainersAboutUser GuideTools

hpcdevops

hpcdevops/singularity-hello-world

DISCUSSIONMAKE PRIVATEBRANCHESEDIT BUILDERDISABLE

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...

SINGULARITYContainersAboutUser GuideTools

hpcdevops

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

Score: 0.6

+

runusrtmplliblocal-scratchetcvarsharesharenotebooks

shareliblocallibinclude

lib

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

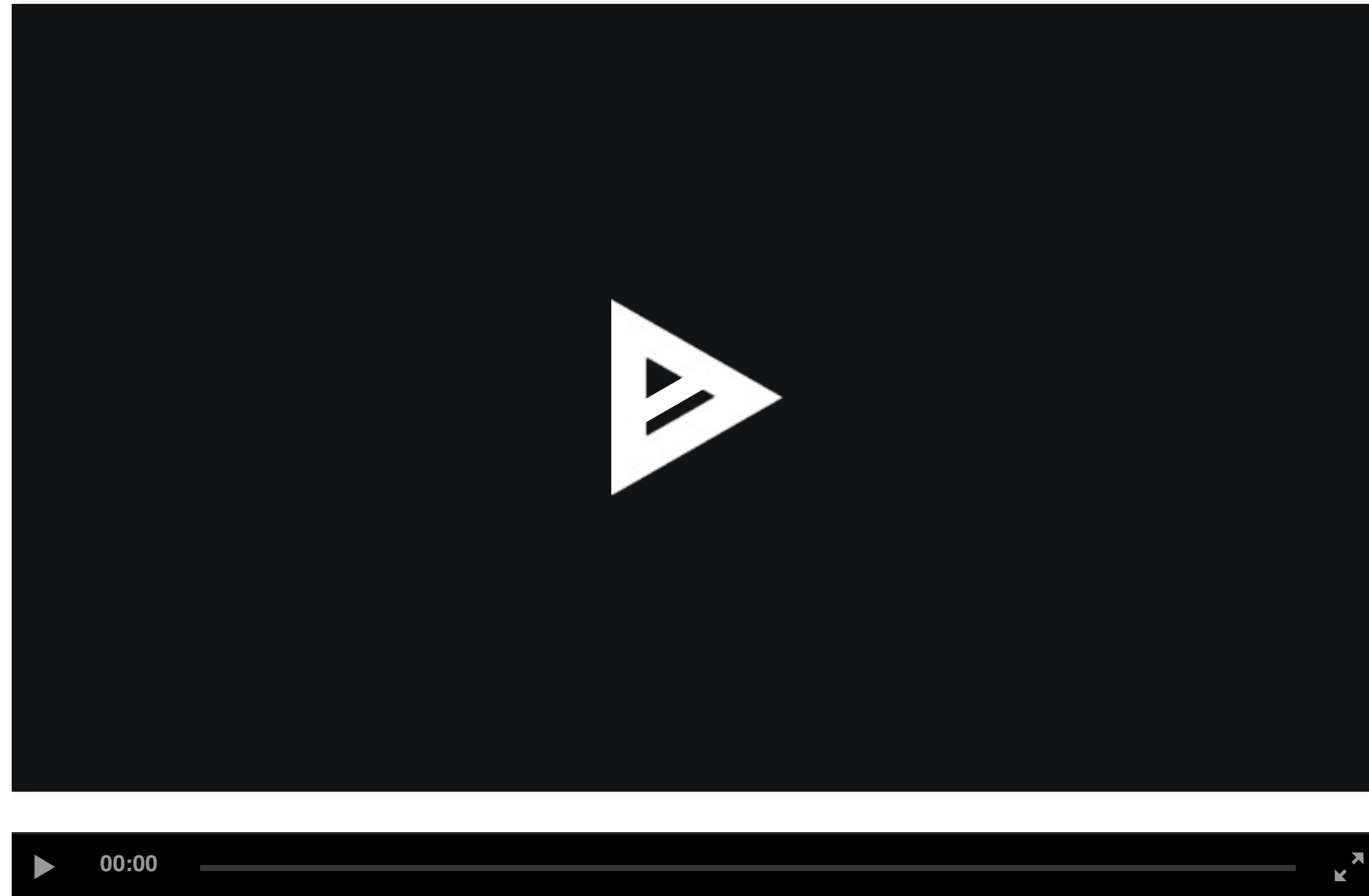
Why to **NOT** use a Virtual Cluster?

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

Installing Cloudmesh Client

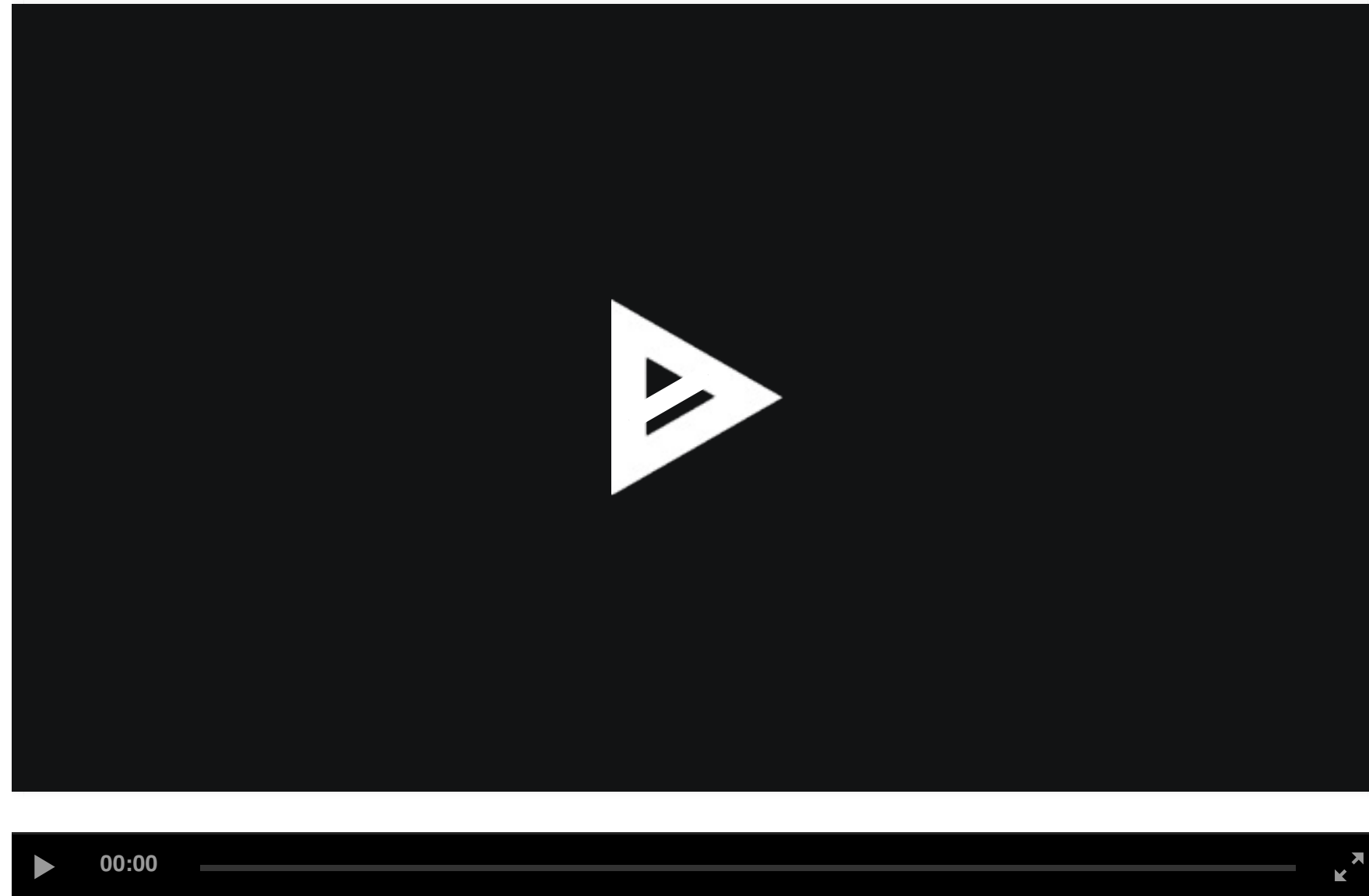
- Create VirtualEnv for Cloudmesh Client
- Install System Dependencies
- Install Cloudmesh Client with pip

Create VirtualEnv for Cloudmesh Client



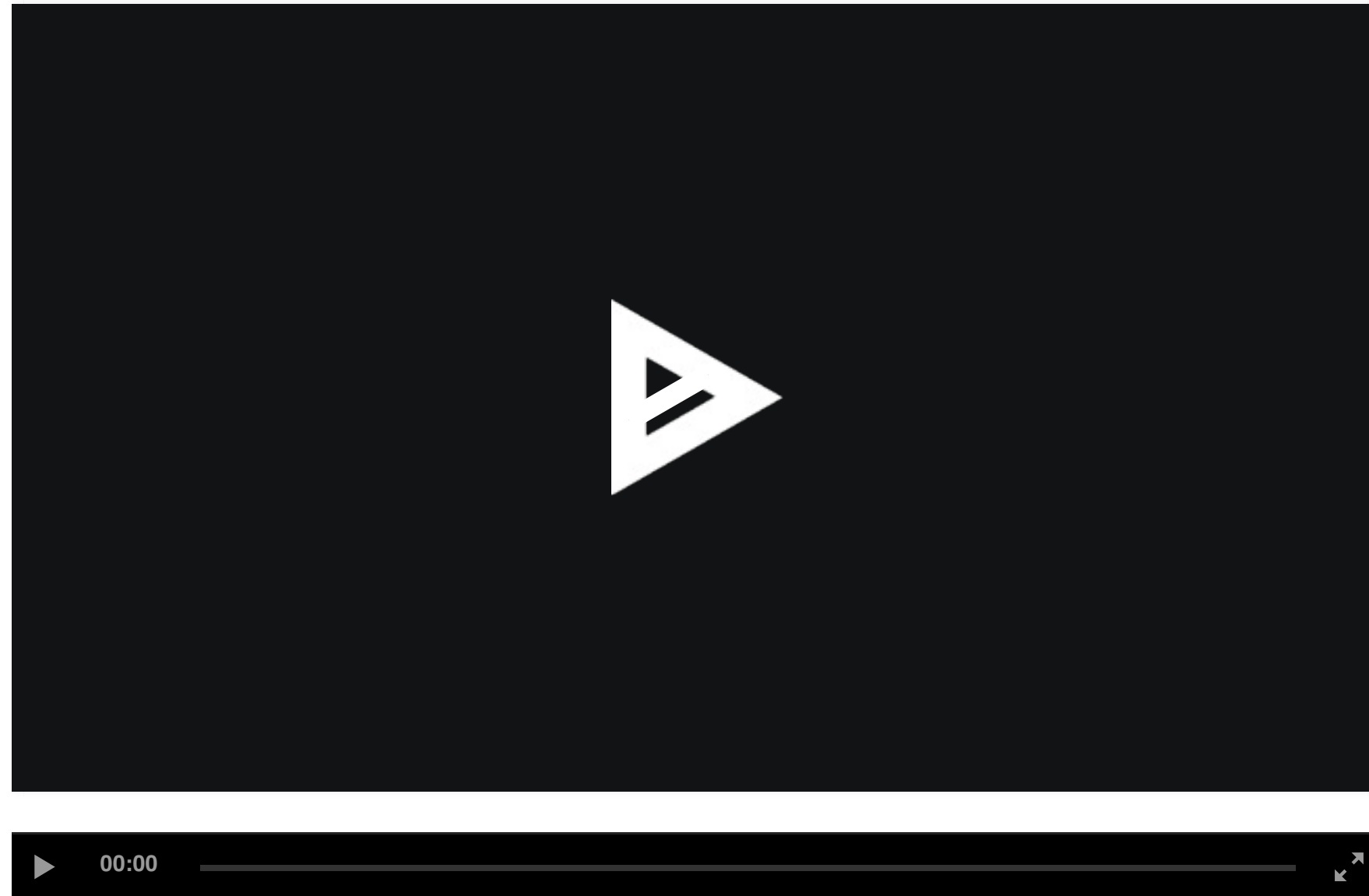
<https://asciinema.org/a/129877>

Install System Dependencies



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

Install Cloudmesh Client with pip



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

Running Cloudmesh Client

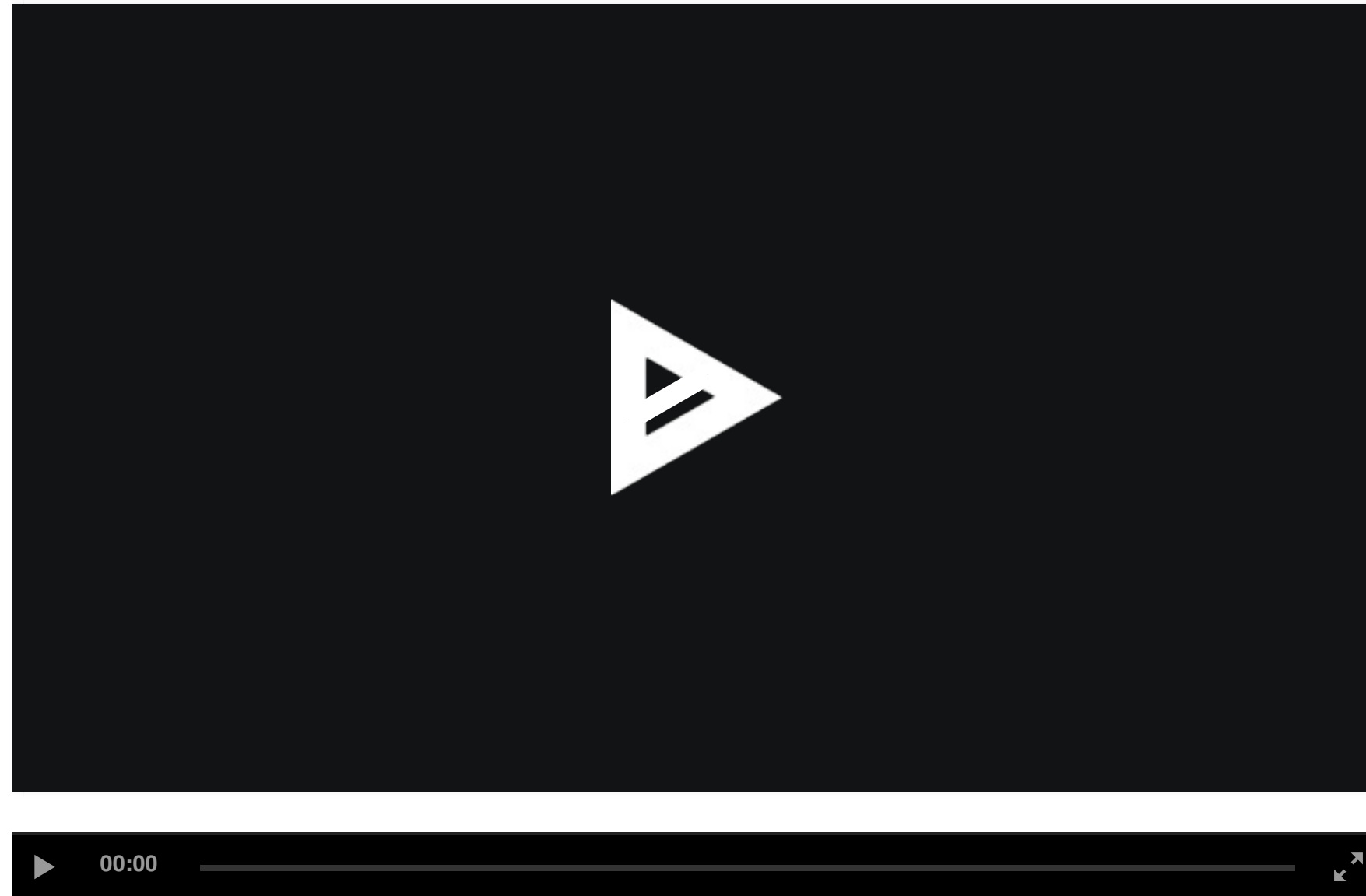
- Initialize Cloudmesh Client
- Virtual Cluster Operations

Initialize Clouddmesh Client



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

Virtual Cluster Operations



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

