



Singularity Containers for Reproducible Workflows

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What is Singularity?



An open-source container runtime born out of the needs of HPC users

Developed by Greg Kurtzer at LBNL from 2015

Now led by Sylabs Inc. and the Singularity community

Allows you to build and run containers on an shared system, without needing to convince your administrator to install docker

Uses existing docker / OCI containers, or create your own Singularity containers



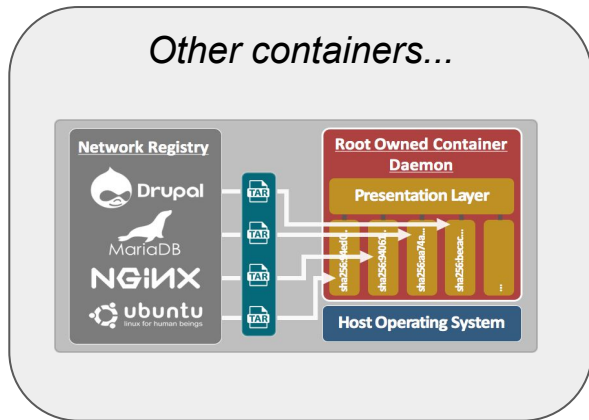
Designed Specifically for Compute



- Drop-in compatibility with nearly every environment
- Native support for: GPUs, Infiniband, MPI, parallel file systems, Cloud and Edge computing
- Optimized for performance and security
 - <https://insidehpc.com/2019/06/benchmarking-mpi-applications-in-singularity-containers-on-traditional-hpc-and-cloud-infrastructures/>
- Blocks privilege escalation within the container
 - Users run as themselves, not root



Singularity Image Format (SIF)



VS



Singularity Image Format (SIF) container provides:

- Single file (no intermediate layers to)
- Immutable base image
- Cryptographic signing & verification
- Reproducibility



The screenshot shows the Sylabs Cloud Singularity Library interface. At the top, there's a navigation bar with 'Home', 'Singularity Library', 'Remote Builder', and 'Keystore'. A search bar is on the right. The main header features the 'Singularity Library' logo and a brief description. Below this, there's a section for 'Share Your Awesome Projects!' with buttons to 'Create a new Project' and 'New Image on existing Project'. A 'Your Recent Activities' section shows a list of recent actions. The main content area displays a list of projects, including 'EMMEFF/TESTBIG1' and 'SEMIQUAN7/WGS_PIPELINE', each with a download button and a size. On the right, there are two sidebars: 'MOST DOWNLOADED' and 'MOST STARRED', each listing popular projects with their respective download counts or star ratings.

Sylabs.io Search Singularity Library...

Home Singularity Library Remote Builder Keystore Help dtrudg-sylabs

Singularity Library

You can find out more about our plans for the library in our [Sylabs lab note](#). Are you looking for additional features, having a problem or would like to provide feedback? Please email us at support@sylabs.io

Share Your Awesome Projects!

Create a new Project New Image on existing Project

Your Recent Activities

- > You created 36 Projects and 54 Images
- > You created 59 Remote Builds
- > You created 2 Keys

EMMEFF/TESTBIG1 Download 1.35 GB

Owner: emmef Description: No description Release Notes: No Description AMD64 STARS: 0 DOWNLOADS: 0

EMMEFF/TESTBIG Download 1.35 GB

Owner: emmef Description: No description Release Notes: No Description AMD64 STARS: 0 DOWNLOADS: 0

Signed With: 02589EC5F53F9027FBF40E4AE17E95A5DF1A124

SEMIQUAN7/WGS_PIPELINE Download 2.11 GB

Owner: semiquan7 Description: WGS PE pipeline

MOST DOWNLOADED

library/alpine	179069
library/busybox	87592
sylabs/not-default	61468
sylabs-bot/testimage1	53547
sylabs-bot/testimage0	53547
sylabs/unsigned	28384
sylabs/signed	14627
library/ubuntu	7886
library/centos	5462
godloved/olcow	3577

MOST STARRED

library/ubuntu	18
library/alpine	14
sylabsd/olcow	11
library/centos	10
library/busybox	8
library/debian	5
sylabs/blender.sif	5
godloved/olcow	4
sylabsd/busybox	2
fempar/fempar	2

Singularity Library

Share containers with others, or keep a private collection.

Tag containers or pull images by hash for reproducibility.

Free service currently offers 11GB quota.



Remote Builder

Singularity 3.0 introduces the ability to build a container in the cloud. Singularity user does not need to prepare an environment or assign permission. Remote Builder can build a container using a provided build definition file

Build a Recipe

Please attach build recipe by dragging & dropping, pasting from the clipboard or [selecting them](#)

```
1 Bootstrap: docker
2 From: alpine:latest
3
4 %runscript
5
6 echo "Hello World!"
```

✓ Build Recipe file is valid

dtrudg-sylabs/default/

Search

Build

Using the Remote Builder from the Singularity CLI

To use the Remote Build Service, first make sure you have a Sylabs cloud token - [get one here](#). Save it to `~/.singularity/sylabs-token`, and then build using the `--remote` flag:

```
singularity build --remote output.sif examples/docker
/Singularity
```

Remote Builder

Build containers in the cloud, when you don't have a Linux machine handy, or can't use root / fakeroot.

Offers a way to ease builds for non-Intel systems.
(On-premise enterprise version)

Free service offers 1,000 build minutes per month (rolling).



Keystore

Singularity (>=3.0) introduced features for signing and verifying SIF™ containers. This ensures a bit-for-bit reproduction of a container. Sylabs Keystore provides an ability to create, manage and use PGP keys in a Singularity container verification workflow

Sign Image

The access token helps Singularity command line identify you to the Singularity Container Services.

You already issued an access token, you are good to go!

[Click here if you want to create a new token.](#)

You need to use Singularity CLI to sign your image locally, you can find the Singularity CLI installation document [here](#)

```
$ singularity sign image.sif
No OpenPGP signing keys found, autogenerate? [Y/n]
Enter your name (e.g., John Doe) : Dave Godlove
Enter your email address (e.g., john.doe@example.com) : d@sylabs.io
Enter optional comment (e.g., development keys) : demo
Generating Entity and OpenPGP Key Pair... Done
Enter encryption passphrase :
```

Verify Image

You need to use the Singularity CLI to verify your image locally, you can find the Singularity CLI installation document [here](#)

✓ Verifying an image is quite easy, just run the verify command within your terminal.

```
$ singularity verify image.sif
Verifying image: image.sif
Data integrity checked, authentic and signed by:
dave <d@sylabs.io>, KeyID 284972D6D4FC6713
```

Search For Keys

🔍 Keys for current signed in user (can search by name or email or fingerprint)

☒ Active ☒ Expired ☒ Expiring

Keys

Name ^	Creation Time ↕	Expiration Time ↕	Algorithm	Bits	Fingerpri
David C. Trudgian (Development Keys) <david.trudgian@sylabs.io>	2019-07-08 10:04:16	Never	rsa	4096	AC0FBD1
David Trudgian (PI3b development keys) <david.trudgian@sylabs.io>	2019-07-18 01:01:44	Never	rsa	4096	86963530

Keystore

Stores public keys against a Sylabs account.

Allow images pulled from the library to be verified as signed by an individual, and unmodified.

Free service



Get Singularity



Open Source: <https://github.com/sylabs/singularity>

For your Mac: <https://sylabs.io/singularity-desktop-macos/>

Paid Supported: <https://sylabs.io/singularity/>

(EPEL for RHEL / CentOS - community packaged, not from Sylabs)



Running a Container



```
02:20 PM $ singularity run library://godlovedc/funny/lolcow
```

```
-----  
/ Your talents will be recognized and \  
\ suitably rewarded.                  /  
-----
```

```
  \      ^      ^  
  \      (oo)\_____  
      (__) \       )\/\  
           ||----w |  
           ||     ||
```

```
02:29 PM $ singularity run docker://dctrud/wttr:latest  
Weather report: Carrollton, United States
```

```
  \      /      Partly cloudy  
- /""'-.      87..91 °F  
  \_ ( ) .    ↑ 11 mph  
 / (___(___)  9 mi  
              0.0 in
```

Thu 10 Oct		
Morning	Noon	Evenin
<pre> \ / Partly cloudy - /""'-. 73..77 °F _ () . ↑ 13-16 mph / (___(___) 6 mi 0.0 in 51%</pre>	<pre> \ / Light rain sho... - /""'-. 77..80 °F _ () . ↑ 14-18 mph / (___(___) 6 mi 0.0 in 72%</pre>	<pre> \ / Thu - /""'-. 84. _ () . ↑ 1 / (___(___) 5 m ⚡ ⚡ ⚡ 0.0</pre>



Accessing the Host's GPU With Tensorflow



```
$ singularity exec --nv docker://tensorflow/tensorflow:latest-gpu python
Python 2.7.12 (default, Dec  4 2017, 14:50:18)
[GCC 5.4.0 20160609] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow as tf
>>> x1 = tf.constant([1,2,3,4])
>>> x2 = tf.constant([5,6,7,8])
>>> result = tf.multiply(x1, x2)
>>> print(result)
Tensor("Mul:0", shape=(4,), dtype=int32)
>>> exit()
$
```



Pulling a Container



```
02:32 PM $ singularity pull library://godlovedc/funny/lolcow
WARNING: Container might not be trusted; run 'singularity verify lolcow_latest.sif' to show who signed it
INFO:      Download complete: lolcow_latest.sif
```

```
02:32 PM $ singularity verify lolcow_latest.sif
Container is signed by 1 key(s):

Verifying signature F: 4426F6CBCB38449E062940A42E6A34D6F54EBE59:
[REMOTE] Dave Godlove (this is the best key) <d@sylabs.io>
[OK]      Data integrity verified

INFO:      Container verified: lolcow_latest.sif
```



Running from a SIF



```
02:32 PM $ singularity run lolcow_latest.sif
```

```
-----  
/ Your lucky number has been \  
\ disconnected. /  
-----
```

```
      ^  ^  
      --  
      (oo)\  
      ( _ )\      )\\  
      | |-----w |  
      | |      | |
```



Building from Docker to SIF



```
02:35 PM $ singularity build wttr.sif docker://dctrud/wttr:latest
INFO:      Starting build...
Getting image source signatures
Skipping fetch of repeat blob sha256:4a56a430b2bac33260d6449e162017e2b23076c6411
a17b46db67f5b84dde2bd
Skipping fetch of repeat blob sha256:82177f28f44660a30bd8a207c5b88b83c4be2329e71
f92ad01f50febe1cf9caf
23076c6411a17b46db67f5b84dde2bd
2019/10/10 14:35:42  info unpack layer: sha256:82177f28f44660a30bd8a207c5b88b83c
4be2329e71f92ad01f50febe1cf9caf
2019/10/10 14:35:42  info unpack layer: sha256:83a1cd2c9d1841681590aa66db329ade6
2a159dc0fa8f88534d8400861c6695d
INFO:      Creating SIF file...
INFO:      Build complete: wttr.sif
```



Building from Docker to SIF



```
02:36 PM $ singularity run wttr.sif
Weather report: Carrollton, United States
```

```
\ /      Partly cloudy
- /"".-.  87..91 °F
 \_( ).   ↑ 11 mph
/(___(___) 9 mi
          0.0 in
```

Thu 10 Oct		
Morning	Noon	Evening
<pre>\ / Partly cloudy - /"".-. 73..77 °F _(). ↑ 13-16 mph /(___(___) 6 mi 0.0 in 51%</pre>	<pre>\ /"".-. Light rain sho... , _(). 77..80 °F /(___(___) ↑ 14-18 mph 6 mi 0.0 in 72%</pre>	<pre>\ /"".-. Thundery outbr... , _(). 84..87 °F /(___(___) ↑ 14-19 mph 5 mi 0.0 in 0%</pre>



Building from a Definition File



```
Bootstrap: docker
```

```
From: debian:buster
```

```
%post
```

```
    apt-get update
```

```
    apt-get -y install curl
```

```
%runscript
```

```
    curl -s https://wttr.in
```



Building from a Definition File



Bootstrap: docker



Where to get our base container

From: debian:buster



What base container to use

%post

apt-get update

apt-get -y install curl



Things to do during the build

%runscript

curl -s https://wttr.in



What happens when we 'run'



Building from a Definition File



```
03:07 PM $ sudo singularity build wttr_demo.sif wttr_demo.def
INFO: Starting build...
Getting image source signatures
Copying blob sha256:4a56a430b2bac33260d6449e162017e2b23076c6411a17b46db67f5b84dde2bd
 48.05 MiB / 48.05 MiB [=====] 1s
Copying config sha256:9bd428a1eab6d94769f7e0d126c07a3b4170e53868e18a7c073ab785fb9b3a39
 579 B / 579 B [=====] 0s
Writing manifest to image destination
Storing signatures
2019/10/10 15:07:58 info unpack layer: sha256:4a56a430b2bac33260d6449e162017e2b23076c6
INFO: Running post scriptlet
+ apt-get update
Get:1 http://cdn-fastly.deb.debian.org/debian buster InRelease [122 kB]
Get:2 http://security-cdn.debian.org/debian-security buster/updates InRelease [30.1 kB]
```

- fakeroot if you don't have sudo / root (requires user namespace)
- remote if you need a remote build in the cloud



Sign..... and Verify



```
03:30 PM $ singularity sign wttr_demo.sif
Signing image: wttr_demo.sif
Enter key passphrase :
Signature created and applied to wttr_demo.sif
```

```
03:31 PM $ singularity verify wttr_demo.sif
Container is signed by 1 key(s):

Verifying signature F: 8C1158660B83F0AFEF7B1D5F91A6ECB189A8F00C:
[LOCAL] David Trudgian (Piran Keys) <dave@trudgian.net>
[OK] Data integrity verified

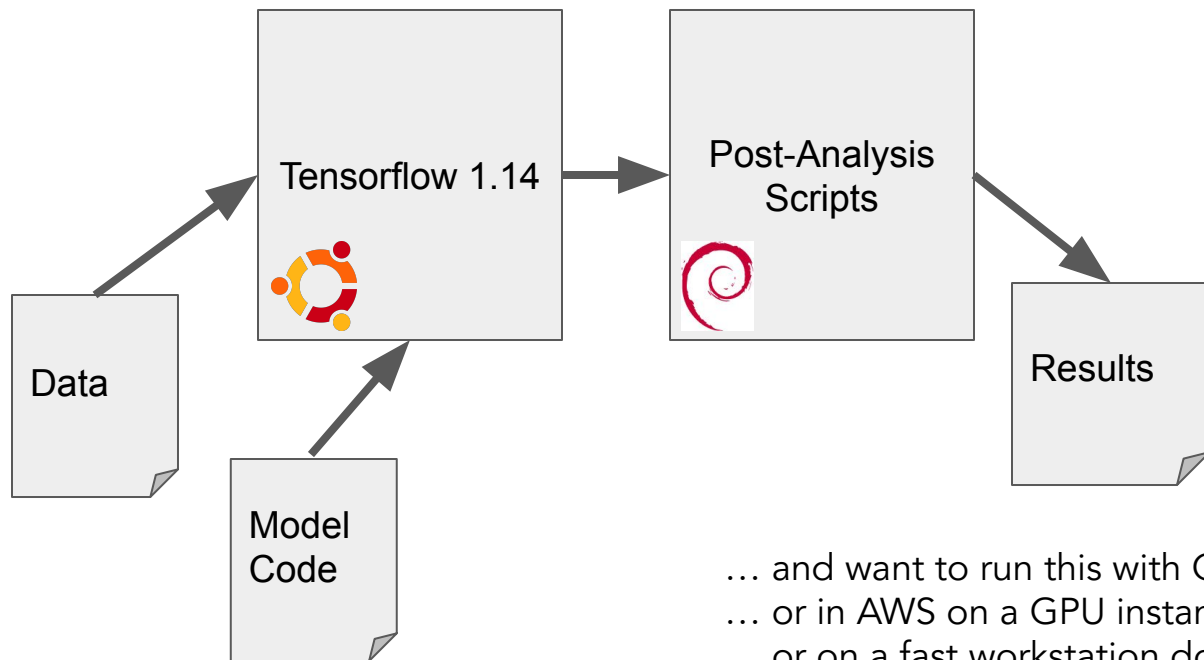
INFO: Container verified: wttr_demo.sif
```



A Simple Workflow



I need to run a tensorflow model, and some scripts I know work on my Debian VM...



... and want to run this with GPUs on a older CentOS 6 cluster
... or in AWS on a GPU instance
... or on a fast workstation down the hall



A Simple Workflow



Prepare...

```
singularity pull tflow114.sif docker://tensorflow/tensorflow:1.14.0-gpu  
sudo singularity build myscripts.sif myscripts.def
```

Copy the containers and data to the cluster, then simply run / submit 2 lines:

```
singularity run --nv tflow114.sif mymodel.py mydata.in  
singularity run myscripts.sif mymodel.out
```

Keep the containers and your data, and you can run it again, reproducibly & easily.

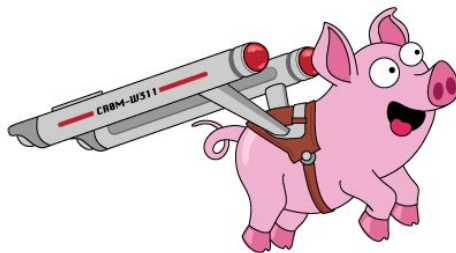


Workflow Tool Integrations



Native support for using Singularity containers in:

nextflow



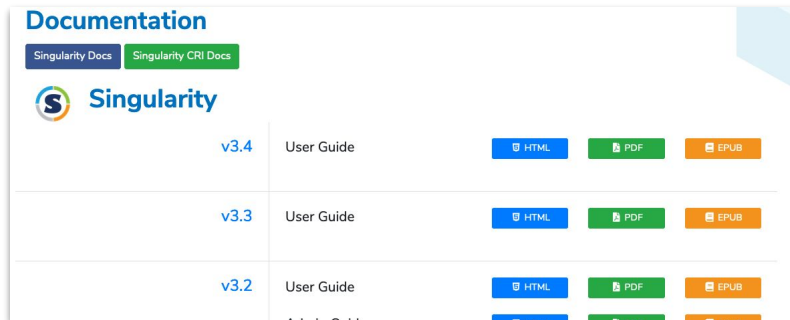
COMMON
WORKFLOW
LANGUAGE

(cwltool, toil)

Snakemake

Documentation & Examples

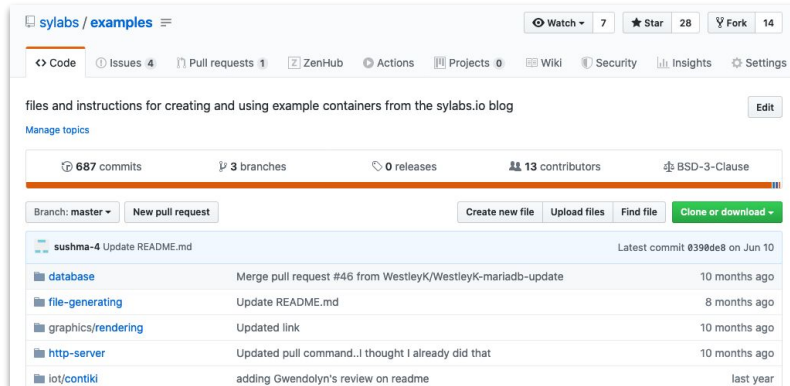
<https://sylabs.io/docs/>



The screenshot shows the Singularity documentation website. At the top, there are tabs for 'Singularity Docs' and 'Singularity CRI Docs'. Below the tabs is the Singularity logo. A table lists documentation for versions v3.4, v3.3, and v3.2. Each version has a 'User Guide' link and buttons for downloading the documentation in HTML, PDF, and EPUB formats.

Version	Documentation Type	HTML	PDF	EPUB
v3.4	User Guide	HTML	PDF	EPUB
v3.3	User Guide	HTML	PDF	EPUB
v3.2	User Guide	HTML	PDF	EPUB

<https://github.com/sylabs/examples>



The screenshot shows the GitHub repository page for 'sylabs/examples'. The page includes a header with navigation links (Code, Issues, Pull requests, ZenHub, Actions, Projects, Wiki, Security, Insights, Settings) and repository statistics (687 commits, 3 branches, 0 releases, 13 contributors, BSD-3-Clause license). Below the header, there is a section for 'Manage topics' and a list of recent commits. The latest commit is 'sushma-4 Update README.md' from Jun 10.

Repository: sylabs / examples

Statistics: 687 commits, 3 branches, 0 releases, 13 contributors, BSD-3-Clause

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

Latest commit: sushma-4 Update README.md on Jun 10

Commit	Description	Time
sushma-4	Update README.md	10 months ago
database	Merge pull request #46 from WestleyK/WestleyK-mariadb-update	10 months ago
file-generating	Update README.md	8 months ago
graphics/rendering	Updated link	10 months ago
http-server	Updated pull command..I thought I already did that	10 months ago
iot/contiki	adding Gwendolyn's review on readme	last year



Community Resources



<https://sylabs.io/resources/community>

Slack



Join Us On Slack

Google Group



Join Google Group

GitHub



Singularity GitHub

Sylabs Twitter



Follow Sylabs On Twitter

Singularity Twitter



Follow Singularity On Twitter

StackOverflow



Singularity On StackOverflow



Questions?



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