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FUEL YOUR INSIGHT

## Containers for Science, Reproducibility and Mobility

# SINGULARITY


Presented By:

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**http://singularity.lbl.gov/**

# CONTAINERS . . .

# CONTAINERS IN HPC: SINGULARITY

# CONTAINERS: WHAT ARE THEY?

In a nutshell:

Containers are encapsulations of system environments

...

(and a means to use it)

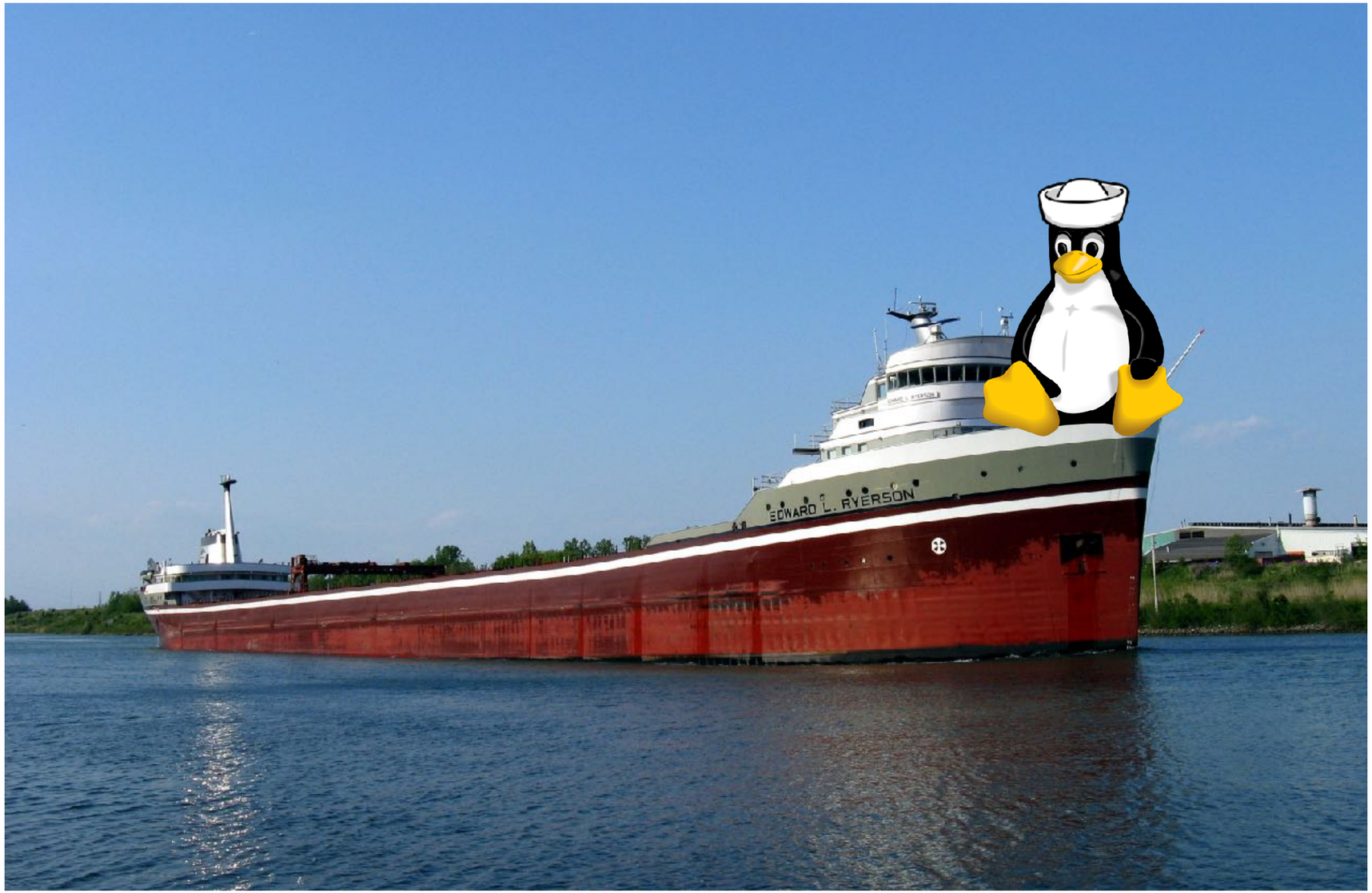
# CONTAINERS IN HPC: SINGULARITY


ubuntu
POWERED BY APACHE
NGINX
http server
PostgreSQL
MariaDB
CentOS

# HOW DOES INDUSTRY MAKE USE OF CONTAINERS?

# CONTAINERS IN HPC: SINGULARITY

# CONTAINERS IN HPC: SINGULARITY



# CONTAINERS IN HPC: SINGULARITY

# CONTAINERS IN HPC: SINGULARITY

# CONTAINERS IN HPC: SINGULARITY

# BUT WHAT ABOUT SCIENCE?

# WHAT IS THE SCIENTIFIC USE CASE?

# CONTAINERS: PRIMARY USE CASES

- Reproducibility!
- Extreme mobility of compute (portability)
- Provides the users, developers and engineers FREEDOM!
  - Can easily leverage other people's work
  - Changes the software distribution and dependency paradigm
  - Depending on application and use-case, simple extreme scalability
  - Containers are in many ways the next logical progression from virtual machines

# CONTAINERS: DOCKER

- Docker is the most well known container platform
- Designed for network service virtualization
- Facilitates workflow of creating, maintaining and distributing containers
- Containers are highly reproducible
- Scientists have jumped on the bandwagon because it seems to have solved their requirements
- User demand is high, interest is high, buzzworthiness is very high!

# SO WHY DON'T WE SEE HPC CENTERS INTEGRATING DOCKER ON THEIR RESOURCES?

# DOCKER IN HPC: THE PROBLEM

- Docker emulates a virtual machine in many aspects (e.g. users can escalate to root)
- Non-authorized users having root access to any of our production networks is considered a security breech
  - To mitigate this security issue, networks must be isolated for Docker access
  - Precludes access to InfiniBand high performance networks and optimized storage platforms
  - Typical solution is a virtual cluster within a physical cluster, but without high performance-ness (removed HP from HPC leaving just C)
- Docker uses a root owned daemon that users can control by means of a writable socket (users control root process)?!
  - What ACLs are in place, are they enough to trust? Can we control or fine tune them?
- No native GPU support. We need to hack Docker, or/also integrate Docker-Nvidia?
- No reasonable support or timeline for MPI… MPI developers estimate this milestone for at least 2 years from now!
- Can not limit access to local file systems, especially when user can achieve root inside container, this breaks all file locally mounted file system security
- Doesn’t support production distributions/kernels (RHEL7 not even completely supported yet)!
- Incompatibilities with existing scheduling and resource manager paradigms:
  - Root owned Docker daemon is outside the reach and control of the resource manager
  - MPI/parallel job runs become increasingly complex due to virtual ad-hoc networking assignments
- Docker is built, maintained, and emphasized for the enterprise, not HPC
- Patches to help make Docker/runC/RKT a better solution for HPC have been submitted … but most have not been accepted!

# DOCKER IN HPC: SUMMARY

Lots of technical implementation problems!

The buzz around Docker on HPC is years old and scientists have been begging, but no HPC centers have integrated a full featured Docker solution on their traditional HPC systems.

HPC is not the appropriate use-case or interest for the Docker community

# SO… WHAT IS THE NEED?

- Reproducibility and archival software and environment stacks
- Mobility of Compute (portable, sharable, distributable container images)
- User defined and controlled environments (BYOE)
- Integratable with existing shared infrastructures and scheduling subsystems
- Properly make use of the existing high performance physical hardware
- Must support running as the user to facilitate scheduling and MPI workflows
- Make use of all of the work that has been done in Docker so far
- We needed it yesterday (so it must be compatible with today's technology)!

# SINGULARITY: HELLO WORLD.

# SINGULARITY DESIGN GOALS

- Architected specifically for scientific reproducibility, “Mobility of Compute” and HPC
- Single file based container images: facilitates modification, distribution, and execution
- No sys-admin, architectural or workflow changes necessary to run Singularity
- Compatibility with existing shared/multi-tenant computational resources
- Maintain user credentials (inside user == outside user)
- Separation between the container and the host can be blurred to leverage host’s resources
- We don’t have to virtualize everything, we can pick and choose as needed

# HOW DOES IT WORK?

# SINGULARITY: PERMISSIONS, ACCESS AND PRIVILEGE

User contexts are always maintained when the container is launched (if it is launched by a particular user, the programs inside will be running as that user) with no escalation pathway within the container! Thus….

If you want to be root inside of the container,

you must first be root outside of the container

# SINGULARITY: WORKFLOW

**End Point the User Controls**

**Root/Superuser**

- Create a new container
- Bootstrap/install container
- System (container) modifications

*Copy image*

*Share image*

**Shared Computational Resource**

**Regular User**

- singularity shell …
- singularity exec …
- singularity run …

# SINGULARITY: CREATE THE CONTAINER

$ sudo singularity create —size 2048 /tmp/Centos-7.img

# SINGULARITY: BOOTSTRAP/INSTALL THE CONTAINER

$ sudo singularity bootstrap /tmp/Centos-7.img centos.def

# SINGULARITY: NOW WE HAVE A CONTAINER…

$ singularity shell /tmp/Centos-7.img

$ singularity exec /tmp/Centos-7.img echo “Hello World”

$ singularity run /tmp/Centos-7.img

# SINGULARITY: LAUNCHING A CONTAINER

- Singularity sets up the container environment and creates the necessary namespaces and execv()s the application(s) within the container
- All expected I/O is passed through the container: pipes, program arguments, stdout, stdin, stderr and X11
- Directories, files and other resources are shared from the host into the container (as allowed by the system administrator)
- When the application(s) finish their foreground execution process, the container and namespaces collapse and vanish cleanly

# SINGULARITY: A PEEK INTO THE CONTAINER

```
$ singularity shell /tmp/Centos-7.img
Singularity: Invoking an interactive shell within container...

Singularity.Centos-7.img> cat /etc/redhat-release
CentOS Linux release 7.2.1511 (Core)
```

# SINGULARITY: MODIFY CONTAINER

```
$ sudo singularity shell —writable /tmp/Centos-7.img
Singularity: Invoking an interactive shell within container...

Singularity.Centos-7.img> yum install …
```

# SINGULARITY: COPY MY PROGRAMS INTO CONTAINER

```
$ sudo singularity copy /tmp/Centos-7.img script.py /usr/bin/

$ singularity exec /tmp/Centos-7.img /usr/bin/script.py
```

# SINGULARITY: EXTREME MOBILITY AND PORTABILITY

# SINGULARITY: EXTREME MOBILITY AND PORTABILITY

# SINGULARITY: CONTAINER IS ALWAYS THE SAME ON THE INSIDE

```
$ singularity shell /tmp/Centos-7.img
Singularity: Invoking an interactive shell within container...

Singularity.Centos-7.img> cat /etc/redhat-release
CentOS Linux release 7.2.1511 (Core)
```

# SINGULARITY: ARCHIVING THE CONTAINER

```
$ gzip -c9 /tmp/Centos-7.img > /tmp/Centos-7.img.gz

$ ls -l /tmp/Centos-7.img /tmp/Centos-7.img.gz
-rwxr-xr-x. 1 root root 805306399 Oct 5 11:14 /tmp/Centos-7.img
-rw-rw-r--. 1 gmk gmk 163498872 Oct  5 14:43 /tmp/Centos-7.img.gz

$ gdrive upload /tmp/Centos-7.img.gz
```

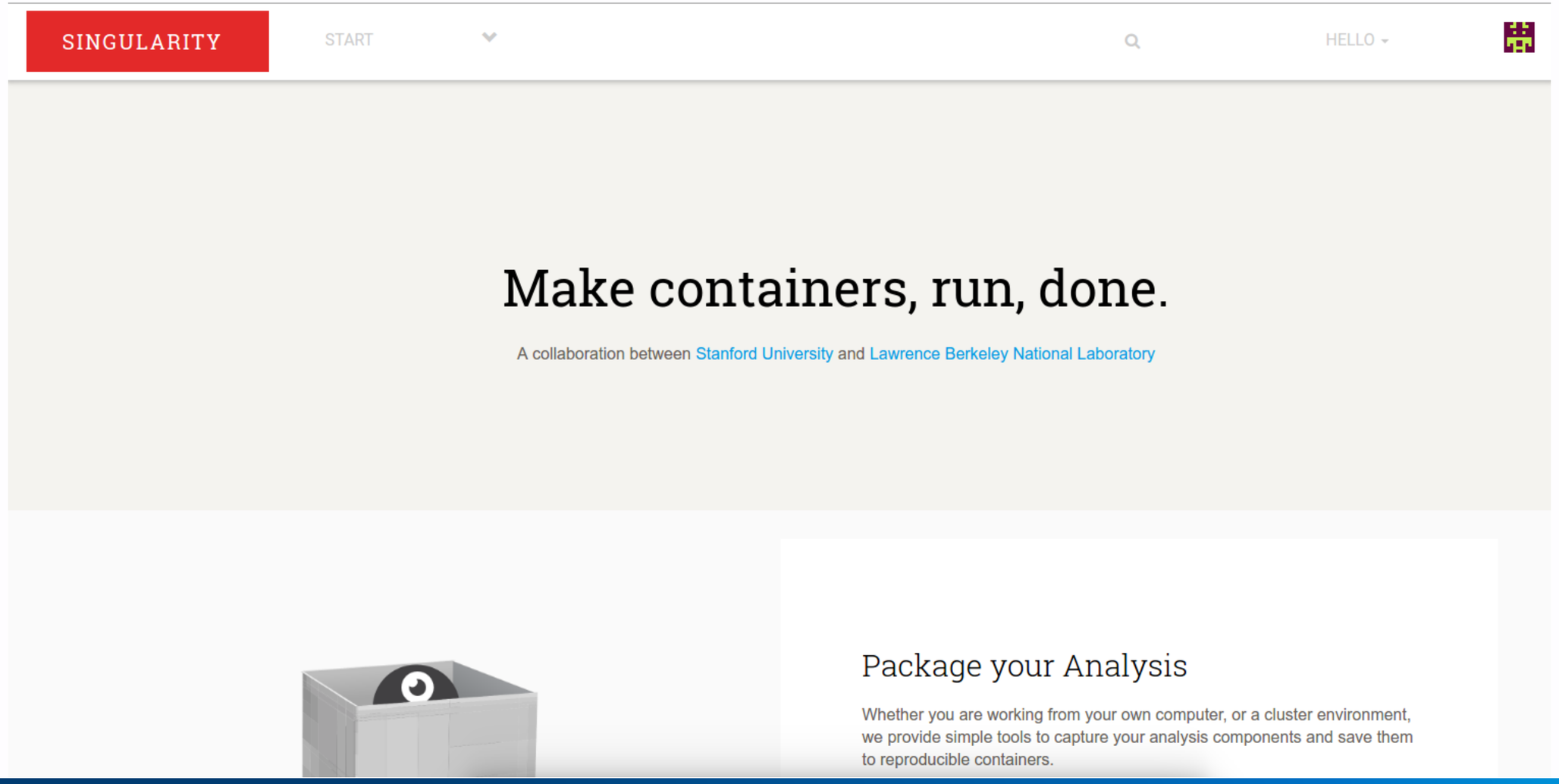
# SINGULARITY VERSION 2.2 IS AVAILABLE NOW!

## HTTP://SINGULARITY.LBL.GOV/

# SINGULARITY: WHO'S USING IT / NAME DROPS / BANDWAGON

- Texas Advanced Computing Center: 462,462 cores / Stampede
- GSI Helmholtz Center for Ion Research: 300,000 cores / GreenCube
- National Institute of Health: 54,000 cores / Biowulf
- UFIT Research Computing at University of Florida: 51,000 cores / HiPerGator
- San Diego Supercomputing Center: 50,000 cores / Comet and Gordon
- Lawrence Berkeley National Laboratory: 30,000 cores / Lawrencium
- Holland Computing Center at UNL/LHC: 14,000 cores / Crane and Tusker

# SINGULARITY HUB: REPRODUCIBLE SCIENCE EXPOSED!



# QUESTIONS?

# INTRODUCTION TO SINGULARITY WORKSHOP (1)

# HTTPS://GITHUB.COM/SINGULARITYWARE/INTEL-HPC-DEVCON

# INTRODUCTION TO SINGULARITY WORKSHOP

# HTTPS://GITHUB.COM/SINGULARITYWARE/INTEL-HPC-DEVCON

# LOG INTO AWS COMPUTE INSTANCES

# (THANK YOU AMAZON!)

# INSTALLATION OF SINGULARITY

# SINGULARITY: INSTALLATION

```
$ sudo yum groupinstall “Development Tools”

$ mkdir ~/git
$ cd ~/git

$ git clone https://github.com/singularityware/singularity.git
$ cd singularity
$ ./autogen.sh
$ ./configure
$ make dist

$ rpmbuild -ta singularity-2.2.tar.gz
$ sudo yum install $HOME/rpmbuild/RPMS/x86_64/singularity-2.2-0.1.el7.centos.x86_64.rpm
```

# SINGULARITY: CONTAINER TEST FROM DOCKER HUB

```
$ singularity shell docker://ubuntu:latest
library/ubuntu:latest
Downloading layer: sha256:a3ed95caeb02ffe68cdd9fd84406680ae93d633cb16422d00e8a7c22955b46d4
Downloading layer: sha256:668604fde02e75dddb4b44c80d4ce20baaac4832c41c3a945f4a236cd7d2f164
Downloading layer: sha256:2879a7ad31445fe2cea410b8ba76704003c11ee05c0a4d32d1113009ea1a1aae
Downloading layer: sha256:de413bb911fd848383ef2e5068a42c258c898d6ee869fb441fb2391eb327b576
Downloading layer: sha256:fc19d60a83f11bbddc7bd2dfca6095b49100314bfde61d83729112a6b6e11d48
Downloading layer: sha256:6bbedd9b76a496816d86a0af731ea984f40467ef8fb23be752f801cb80436ac6
Singularity: Invoking an interactive shell within container…

Singularity.ubuntu:latest> cat /etc/lsb-release
DISTRIB_ID=Ubuntu
DISTRIB_RELEASE=16.04
DISTRIB_CODENAME=xenial
DISTRIB_DESCRIPTION="Ubuntu 16.04.1 LTS”
Singularity.ubuntu:latest> which apt-get
/usr/bin/apt-get
Singularity.ubuntu:latest> exit
```

# CREATING/BOOTSTRAPPING A NEW CONTAINER

# SINGULARITY: BOOTSTRAP DEFINITION/RECIPE

```
$ cat examples/debian.def
# Copyright (c) 2015-2016, Gregory M. Kurtzer. All rights reserved.
#
# "Singularity" Copyright (c) 2016, The Regents of the University of California,
# through Lawrence Berkeley National Laboratory (subject to receipt of any
# required approvals from the U.S. Dept. of Energy).  All rights reserved.

BootStrap: debootstrap
OSVersion: stable
MirrorURL: http://ftp.us.debian.org/debian/

%runscript
    echo "This is what happens when you run the container..."

%post
    echo "Hello from inside the container"
    apt-get update
    apt-get -y install vim
```

# SINGULARITY: NEW IMAGE CREATION

```
$ sudo singularity create /tmp/Debian.img
Creating a new image with a maximum size of 768MiB...
Executing image create helper
Formatting image with ext3 file system
Done.

$ ls -l /tmp/Debian.img
-rwxr-xr-x. 1 root root 805306399 Nov  5 07:22 /tmp/Debian.img

$ /tmp/Debian.img
ERROR  : Container does not have a valid /bin/sh
ABORT  : Retval = 255
```

# SINGULARITY: BOOTSTRAP

```
$ sudo singularity bootstrap /tmp/Debian.img examples/debian.def
Bootstrap initialization
Checking bootstrap definition
Executing Prebootstrap module
Executing Bootstrap 'debootstrap' module
… snip …
Processing /usr/share/vim/addons/doc
Setting up vim (2:7.4.488-7) ...
update-alternatives: using /usr/bin/vim.basic to provide /usr/bin/vim (vim) in auto mode
update-alternatives: using /usr/bin/vim.basic to provide /usr/bin/vimdiff (vimdiff) in auto mode
update-alternatives: using /usr/bin/vim.basic to provide /usr/bin/rvim (rvim) in auto mode
update-alternatives: using /usr/bin/vim.basic to provide /usr/bin/rview (rview) in auto mode
update-alternatives: using /usr/bin/vim.basic to provide /usr/bin/vi (vi) in auto mode
update-alternatives: using /usr/bin/vim.basic to provide /usr/bin/view (view) in auto mode
update-alternatives: using /usr/bin/vim.basic to provide /usr/bin/ex (ex) in auto mode
update-alternatives: using /usr/bin/vim.basic to provide /usr/bin/editor (editor) in auto mode
Processing triggers for libc-bin (2.19-18+deb8u6) ...
Done.
```

# USING THE CONTAINERS

# SINGULARITY: USING YOUR NEW CONTAINER

```
$ singularity shell /tmp/Debian.img
Singularity: Invoking an interactive shell within container...

Singularity.Debian.img> uname -a
Linux ip-172-31-20-175 3.10.0-327.28.2.el7.x86_64 #1 SMP Wed Aug 3 11:11:39 UTC 2016 x86_64 GNU/
Linux
Singularity.Debian.img> whoami
gmk
Singularity.Debian.img> pwd
/home/gmk/git/singularity
Singularity.Debian.img> ./configure
checking build system type... x86_64-unknown-linux-gnu
checking host system type... x86_64-unknown-linux-gnu
checking target system type... x86_64-unknown-linux-gnu
checking for a BSD-compatible install... /usr/bin/install -c
… snip …
configure: error: in `/home/gmk/git/singularity':
configure: error: no acceptable C compiler found in $PATH
See `config.log' for more details
Singularity.Debian.img> exit
```

# SINGULARITY: USING YOUR NEW CONTAINER

```
$ singularity exec /tmp/Debian.img uname -a
Linux ip-172-31-20-175 3.10.0-327.28.2.el7.x86_64 #1 SMP Wed Aug 3 11:11:39 UTC 2016 x86_64 GNU/
Linux
$ singularity exec /tmp/Debian.img whoami
gmk
$ singularity exec /tmp/Debian.img pwd
/home/gmk/git/singularity
$ singularity exec /tmp/Debian.img ./configure
checking build system type... x86_64-unknown-linux-gnu
checking host system type... x86_64-unknown-linux-gnu
checking target system type... x86_64-unknown-linux-gnu
checking for a BSD-compatible install... /usr/bin/install -c
… snip …
configure: error: in `/home/gmk/git/singularity':
configure: error: no acceptable C compiler found in $PATH
See `config.log' for more details
$ singularity run /tmp/Debian.img
This is what happens when you run the container...
$ /tmp/Debian.img
This is what happens when you run the container...
```

# SINGULARITY: USAGE AND OPTION EXAMPLES

```
# Notice the PS output is now in a new process namespace
$ singularity exec -p /tmp/Debian.img ps auxf

# What happens when Contained? Create some files in your home, are they persistent?
$ singularity shell --contain /tmp/Debian.img

# Contain but define a new directory to use for your home
$ singularity shell --contain --home ~/git /tmp/Debian.img

# User defined bind points. What happens if you specify a bind point that doesn't exist? What
# about if you bind ontop of a system location (e.g. /bin/)?
$ singularity shell --bind /tmp:/opt /tmp/Debian.img

# How is the shell environment transposed into the container?
$ singularity exec /tmp/Debian.img env
$ singularity exec /tmp/Debian.img env | wc -l
$ env -i singularity exec /tmp/Debian.img env | wc -l
$ env -i FOO=BAR singularity exec /tmp/Debian.img env
```

# SINGULARITY: CHANGING YOUR CONTAINER

```
$ singularity exec /tmp/Debian.img python —version
/.exec: line 3: exec: python: not found
$ sudo singularity exec --writable /tmp/Debian.img apt-get -y install python
Reading package lists... Done
Building dependency tree
Reading state information... Done
The following extra packages will be installed:
  file libexpat1 libffi6 libmagic1 libpython-stdlib libpython2.7-minimal libpython2.7-stdlib
libsqlite3-0 libssl1.0.0 mime-support python-minimal python2.7 python2.7-minimal
 … snip …
Setting up libpython-stdlib:amd64 (2.7.9-1) ...
Setting up python (2.7.9-1) ...
Setting up file (1:5.22+15-2+deb8u2) ...
Processing triggers for libc-bin (2.19-18+deb8u6) ...
$ singularity exec /tmp/Debian.img python --version
Python 2.7.9
```

# SINGULARITY: MORE CONTAINER AWESOMENESS

```
$ cat ~/hello.py
#!/usr/bin/python
import sys
print("Hello World: The Python version is %s.%s.%s" % sys.version_info[:3])
$ python ~/hello.py
Hello World: The Python version is 2.7.5
$ singularity exec /tmp/Debian.img python ~/hello.py
Hello World: The Python version is 2.7.9
$ cat ~/hello.py | singularity exec /tmp/Debian.img python
Hello World: The Python version is 2.7.9
$ singularity exec docker://python:latest /usr/local/bin/python ~/hello.py
library/python:latest
Downloading layer: sha256:a3ed95caeb02ffe68cdd9fd84406680ae93d633cb16422d00e8a7c22955b46d4
Downloading layer: sha256:0a587a7fabdab20075256ed13afc7a39228dba7e9aaf0835c10860fe5abc1bd7
Downloading layer: sha256:d96297b6dc069127b12c63f533f253436496380a42c4a48d3702327ab028f275
Downloading layer: sha256:a3ed95caeb02ffe68cdd9fd84406680ae93d633cb16422d00e8a7c22955b46d4
Downloading layer: sha256:a3ed95caeb02ffe68cdd9fd84406680ae93d633cb16422d00e8a7c22955b46d4
 … snip …
Hello World: The Python version is 3.5.2
```

# WORKFLOWS/RUNSCRIPTS

# SINGULARITY: BOOTSTRAP DEFINITION/RECIPE (WITH RUNSCRIPT/WORKFLOW)

```
$ cat examples/debian.def
# Copyright (c) 2015-2016, Gregory M. Kurtzer. All rights reserved.
#
# "Singularity" Copyright (c) 2016, The Regents of the University of California,
# through Lawrence Berkeley National Laboratory (subject to receipt of any
# required approvals from the U.S. Dept. of Energy).  All rights reserved.

BootStrap: debootstrap
OSVersion: stable
MirrorURL: http://ftp.us.debian.org/debian/

%runscript
    for i in $@; do
        grep "$i" /etc/services
    done

%post
    echo "Hello from inside the container"
    apt-get update
    apt-get -y install netbase
```

# SINGULARITY: BOOTSTRAP

```
$ sudo singularity create -F /tmp/Debian-workflow.img
Creating a new image with a maximum size of 768MiB...
Executing image create helper
Formatting image with ext3 file system
Done.
$ sudo singularity bootstrap /tmp/Debian-workflow.img examples/debian.def
Bootstrap initialization
Checking bootstrap definition
Executing Prebootstrap module
Executing Bootstrap 'debootstrap' module
… snip …
Setting up libisccfg-export90 (1:9.9.5.dfsg-9+deb8u6) ...
Setting up libirs-export91 (1:9.9.5.dfsg-9+deb8u6) ...
Setting up iproute2 (3.16.0-2) ...
Setting up ifupdown (0.7.53.1) ...
Creating /etc/network/interfaces.
Setting up isc-dhcp-common (4.3.1-6+deb8u2) ...
Setting up isc-dhcp-client (4.3.1-6+deb8u2) ...
Setting up libxtables10 (1.4.21-2+b1) ...
Setting up netbase (5.3) ...
Processing triggers for libc-bin (2.19-18+deb8u6) ...
Processing triggers for systemd (215-17+deb8u5) ...
Done.
```

# SINGULARITY: EXECUTING THE RUNSCRIPT

```
$ singularity run /tmp/Debian-workflow.img ^http
http            80/tcp          www             # WorldWideWeb HTTP
http            80/udp                          # HyperText Transfer Protocol
https           443/tcp                         # http protocol over TLS/SSL
https           443/udp
http-alt        8080/tcp        webcache        # WWW caching service
http-alt        8080/udp

$ ls -l /tmp/Debian-workflow.img
-rwxr-xr-x. 1 root root 805306399 Nov  5 07:22 /tmp/Debian-workflow.img
$ sudo mv /tmp/Debian-workflow.img /usr/local/bin/service_lookup
$ service_lookup ^ftp ^smtp
ftp-data        20/tcp
ftp             21/tcp
ftps-data       989/tcp                         # FTP over SSL (data)
ftps            990/tcp
smtp            25/tcp          mail
```

# SINGULARITY: EXTREME MOBILITY AND PORTABILITY

# SINGULARITY: TENSORFLOW

```
$ sudo singularity create --size 4096 /tmp/Tensor.img
Creating a new image with a maximum size of 4096MiB...
Executing image create helper
Formatting image with ext3 file system
Done.
$ sudo singularity bootstrap /tmp/Tensor.img examples/contrib/debian85-tensorflow-0.10.def
Bootstrap initialization
Checking bootstrap definition
Executing Prebootstrap module
W: Cannot check Release signature; keyring file not available /usr/share/keyrings/debian-archive-
keyring.gpg
I: Retrieving Release
I: Retrieving Packages
 … snip …
Minibatch loss: 1.603, learning rate: 0.006302
Minibatch error: 0.0%
Validation error: 0.9%
Test error: 0.8%
Done.
```

# SINGULARITY: TENSORFLOW

```
$ cat examples/contrib/debian85-tensorflow-0.10.def
BootStrap: debootstrap
OSVersion: stable
MirrorURL: http://ftp.us.debian.org/debian/


%runscript
    exec /usr/bin/python

%post
    apt-get update
    apt-get -y install vim python-pip python-dev
    pip install --upgrade https://storage.googleapis.com/tensorflow/linux/cpu/tensorflow-0.10.0-
cp27-none-linux_x86_64.whl

%test
    # This runs usually less then 30 minutes depending on your host type
    python -m tensorflow.models.image.mnist.convolutional
```

# DISCUSSION AND QUESTIONS

INTEL® HPC DEVELOPER CONFERENCE

FUEL YOUR INSIGHT

Containers for Science, Reproducibility and Mobility

# SINGULARITY P1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