SINGULARITY

BUILD YOUR SOFTWARE ENVIRONMENT ON YOUR PC

RUN IT ON ANY LINUX MACHINE USING SINGULARITY

16:00
10 May 2017

Donald Smits Room
Smitsborg - Nettelbosje 1
Containers: why, what, which, how?

Live demo
Who...

already knows something about containers?
Who... has ever run a container?
Who... has heard about or used Singularity?
The hype about containers...
What's the hype about?
Installation issues
“Reviewers have asked him to reproduce the experiment.”
Virtual machines?
Virtual machine
Virtual machine vs container
Containers in a nutshell:

"Containers are encapsulations of system environments... (and a means to use it)"

Gregory Kurtzer, developer of Singularity
https://github.com/singularityware/intel-hpc-devcon
Container features

Freedom: define your own environment

Singularity.ubuntu.img> # apt-get install python3.4
Reading package lists... Done
Building dependency tree
Reading state information... Done
The following extra packages will be installed:
  libmpdec2 libpython3.4-minimal libpython3.4-stdlib python3.4-minimal
Suggested packages:
  python3.4-doc binutils bjinfmt-support
The following NEW packages will be installed:
  libmpdec2 libpython3.4-minimal libpython3.4-stdlib python3.4
python3.4-minimal
0 upgraded, 5 newly installed, 0 to remove and 0 not upgraded.
Need to get 3974 kB of archives.
After this operation, 17.7 MB of additional disk space will be used.
Do you want to continue? [Y/n] Y
Get:1 http://us.archive.ubuntu.com/ubuntu/ trusty/main libmpdec2 amd64 2.4.0-6 [79.4 kB]
Get:2 http://us.archive.ubuntu.com/ubuntu/ trusty/main libpython3.4-minimal amd64 3.4.0-2ubuntu1 [444 kB]
Get:3 http://us.archive.ubuntu.com/ubuntu/ trusty/main libpython3.4-stdlib amd64 3.4.0-2ubuntu1 [205 kB]
Get:4 http://us.archive.ubuntu.com/ubuntu/ trusty/main python3.4-minimal amd64 3.4.0-2ubuntu1 [1273 kB]
Get:5 http://us.archive.ubuntu.com/ubuntu/ trusty/main python3.4 amd64 3.4.0-2ubuntu1 [163 kB]
Fetched 3974 kB in 1s (2249 kB/s)
Container features

Complex installations: only do it once
Container features

Portability / mobility
Container features

Reproducibility
Container features

Performance
Disadvantages

› Overhead:
  › Size
  › Time

› Host dependencies:
  › Container software
  › Kernel
Different container solutions

(and many others...)
Different container solutions

- Docker
- HPC

RIS ACADEMY
I CAN HAS SINGULARITY?
Singularity

- Easy to install and configure
- Easy to run/use:
  - no daemons
  - no root
  - works with scheduling systems
- User outside container == user inside container
- Access to host resources
- Mount (parts of) filesystems of the host
- MPI
Singularity: container formats

› Singularity container format
› Unix directory
› Different compressed formats
   › .tar, .tar.gz, .tar.bz2
   › cpio, cpio.gz

› Supported URIs:
   ○ http://
   ○ https://
   ○ docker://
   ○ shub://
Singularity workflow

**User controlled system**

- Root/superuser
  - Create a new container
  - Bootstrap/install container
  - Modify container

**Shared computational resource**

- Regular user
  - Execute / run container
  - Command line shell in container

- Copy / share image
Singularity hub

https://singularity-hub.org
Build, view, share, deploy, visualize
Use case:

- A user with root access to a Linux system (e.g. Ubuntu Laptop)...
- ... and user access to another Linux system (e.g. Peregrine HPC Cluster)
- Needs to run particular software, which is not easily available on the second system.
- Needs to install/delete several software packages

Solution:

- Package everything in a Singularity container on the Laptop and...
- ... run it on Peregrine
Step 1: Install Singularity in Ubuntu
Step 2: Create a Singularity image
Step 3: Populate the image with an OS (Ubuntu)
Step 3(b): Test the image by shelling in
Step 4: Modify the image
Step 5: Copy the image to Peregrine
Step 6: Run it
Step 7: Go to step 4
Tutorials

› May 16th, 15:00
› Hands-on exercises
› Create and try out your own containers
› More advanced topics

› Register here (only 4 seats left!):
  https://goo.gl/forms/QG4MGtXpHl1prZaQ2
  https://twitter.com/CIT_HPC
More information

› Singularity website: 
http://singularity.lbl.gov

› Singularity Hub: 
https://singularity-hub.org

› Peregrine wiki page: 
https://redmine.hpc.rug.nl

› RIS Academy website: 
http://rug.nl/risacademy