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Containers in HPC: Singularity/Apptainer

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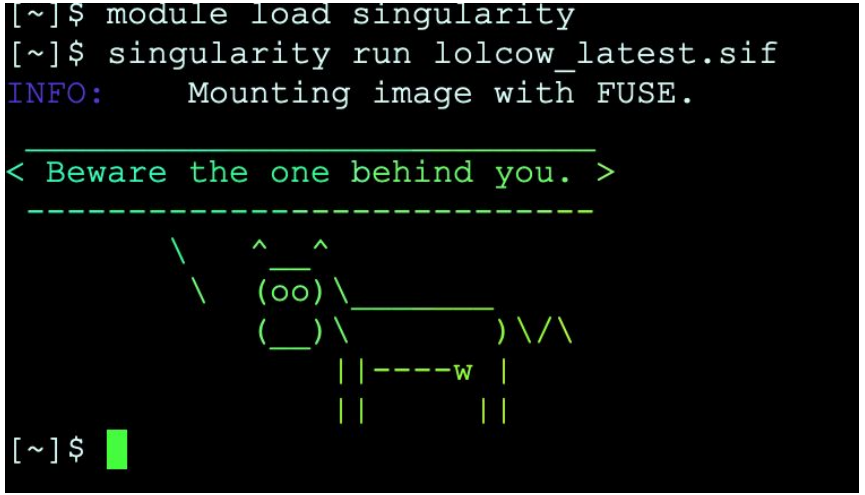
Outline



- What are the containers?
- Using singularity or apptainer
- Lolcow example
- Running lammps on GPUs using singularity and apptainer

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What are the containers?

- ★ Containers are used to bundle an application with all its necessary files into one runtime environment.
- ★ As one unit, a container can easily be moved and run on any operating system in any context.
- ★ Containers isolates software and allows it to work independently across different operating systems, hardware, networks, storage systems, …
- ★ Containers are supposed to make software dependencies management easier.

- ★ Alternative solution for running software: difficult to build from source
- ★ Possibility to convert Docker images to singularity/Apptainer.
- ★ Possibility to build custom containers from definition files.

Using singularity and apptainer

- You will need Singularity/Apptainer engine installed:
  - https://github.com/sylabs/singularity (sources, RPMS)
  - https://github.com/apptainer/apptainer ; also in EPEL
  - Needs root privileges to install

- On the Alliance Federation systems, Apptainer is installed as a module
  [~@yak ~]$ module load apptainer
- On Grex, Singularity-CE is installed as a module
  [~@yak ~]$ module load singularity

- Then, “apptainer” or “singularity” will be in the PATH Lets run a first container?
  [~@yak ~]$ singularity help (or apptainer help)
  [~@yak ~]$ singularity exec library://lolcow cowsay "Mooo"
  [~@yak ~]$ singularity run docker://godlovedc/lolcow (this will work with apptainer)

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Lolcow example

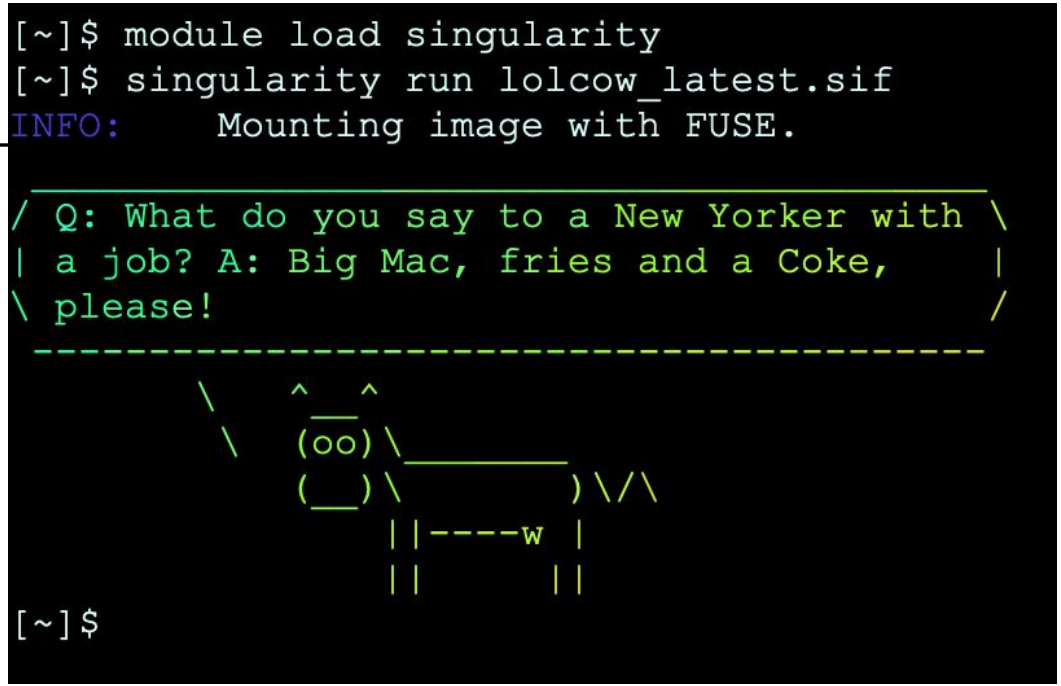
On Grex:

```
[~@yak ~]$  module load singularity
[~@yak ~]$  singularity pull library://sylabsed/examples/lolcow
INFO:    Downloading library image
79.9MiB / 79.9MiB [==========================================] 100 %
9.6 MiB/s 0s
WARNING: integrity: signature not found for object group 1
WARNING: Skipping container verification

[~@yak ~]$  du -sh lolcow_latest.sif
80M     lolcow_latest.sif
```

Lolcow example

```
[~@yak ~]$  module load singularity
[~@yak ~]$  singularity run lolcow_latest.sif
INFO:      Mounting image with FUSE.
 _______________________________________
/ I was gratified to be able to answer \
| promptly, and I did. I said I didn't |
| know.                                |
|                                      |
\ -- Mark Twain                        /
 ---------------------------------------
        \   ^__^
        \  (oo)\_______
        (__)\       )\/\
            ||----w |
            ||     ||
```



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Lolcow example on MC

Run lolcow from docker:

```
[~@ ~]$  module load apptainer
[~@ ~]$  singularity run docker://godlovedc/lolcow
```

Build the image:

```
[~@ ~]$ module load apptainer
[~@ ~]$ singularity pull docker://godlovedc/lolcow
```

Use the existing image:

```
[~@ ~]$ cp /home/shared/ws-may2025/images/lolcow_latest.sif .
[~@ ~]$ module load apptainer
[~@ ~]$ apptainer run lolcow_latest.sif
[~@ ~]$ singularity run lolcow_latest.sif
```

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More commands

```
singularity run lolcow_latest.sif

singularity inspect lolcow_latest.sif

singularity inspect --runscript lolcow_latest.sif

singularity inspect --deffile lolcow_latest.sif

singularity exec lolcow_latest.sif  apt list --installed

singularity exec lolcow_latest.sif  awk 'BEGIN {print "Hello World"}'
```

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Lammps using a container

- How to pull the lammps image?
- How to run the container on MC and Grex?

MC: cp /home/shared/ws-may2025/images/lammps_patch_3Nov2022.sif .
Grex: cp /global/software/ws-may2025/images/lammps_patch_3Nov2022.sif .

MC:

```
salloc --gpus=1 --cpus-per-gpu=1 --mem=8000 --time=1:00:00
module load apptainer
```

Grex:

```
salloc --gpus=1 --cpus-per-gpu=1 --mem=8000 --time=1:00:00
--partition=gpu,stamps-b,livi-b,agro-b
module load singularity
```

```
singularity run --nv -B $PWD:/host_pwd --pwd /host_pwd ./lammps_patch_3Nov2022.sif
./run_lammps.sh
```

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Thank you for your attention

Any question?

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Singularity or Apptainer

- Singularity was developed since 2017 by a company called Sylabs.
  https://sylabs.io/
- Due to personal conflicts, the development got forked to HPC-NG
- Then, HPC-NG was taken as a Linux Foundation project Apptainer.
  https://apptainer.org/
- Sylabs develops Singularity-CE and an Enterprise edition.
- Wikipedia has an interesting discussion
  https://en.wikipedia.org/wiki/Talk:Singularity_(software)
- The teams work in different directions, but so far products are compatible
  - The Container SIF format
  - OverlayFS support, rootless features
  - Support of OCI container format

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Do I need root to build container?

- Yes, in some cases it is still needed.
  - When building new containers
  - Inspecting container images

- Containers have a working copy of an entire Linux distribution, some parts of which are owned by root.
  - Thus to build a new container, one has to be root!
  - Unless a ready image from Docker is usable
  - Unless a system and Singularity/Apptainer installation support fakeroot and namespaces
  - Unless you delegate build of the image to a remote build service

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Singularity/Apptainer

- Can “exec” software from well-built containers images
- Can convert suitably built Docker images
  - Making or finding a suitable container image is a bit of work
  - Bleeding-edge codes usually are poorly maintained and that includes their Docker images
- If software is already provided via Modules-based HPC software stack?
- Encapsulating software and sometimes data to reduce number of files
  - Conda is the prime example
  - OpenFOAM, certain GIS software could benefit from writable overlays

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qiime2

```
[~@yak ~]$  module load singularity
[~@yak ~]$  singularity build qiime2-2023.3.sif docker://quay.io/qiime2/core:2023.2
INFO:     Starting build...
2023/05/15 14:46:02  info unpack layer:
sha256:3f4ca61aafcd4fc07267a105067db35c0f0ac630e1970f3cd0c7bf552780e985
….
INFO:     Creating SIF file…
INFO:     Build complete: qiime2-2023.3.sif

[~@yak ~]$ module load apptainer
[~@yak ~]$ apptainer build qiime2.sif docker://quay.io/qiime2/core:2023.2
```

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More readings

Resources: Github, DockerHub, SingularityHub, Aptainer.

Singularity examples: https://github.com/singularityware/singularity/tree/master/examples

- ★ **Documentation:** https://singularityware.github.io/user-guide.html
- ★ **DockerHub:** https://hub.docker.com/explore/
- ★ **SingularityHub:** https://www.singularity-hub.org/
- ★ **Apptainer:** https://apptainer.org/docs/

https://um-grex.github.io/grex-docs/

Access to Singularity:

- ★ **Connect to cluster:** Grex
- ★ **Load a module:** module load singularity
- ★ **Build the image:** convert the image from Docker to Singularity
- ★ **Note:** You may need to use your own Linux machine or VM to build the image