Magic Tools to Install & Manage Software

Part 2: Singularity Container

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Magic Tools to Install & Manage Software

Part 1: CONDA Virtual Environment

Part 2: Singularity Container

Outlines

1. Why Container?
2. Run an Existing Container Image
3. Get More Container Images
4. Build Your Own Container Image

Outlines

1. **Why Container?**
   1) Problems
   2) Container & Singularity

2. **Run an Existing Container Image**
   1) What you need
   2) Basic commands
   3) Running jobs with Singularity

3. **Get More Container Images**
   1) What you need
   2) Where to get
   3) How to get

4. **Build Your Own Container Image**
   1) What you need
   2) Typical workflow
   3) Make it easier - Recipe

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1) Problems

- **Core problem:**

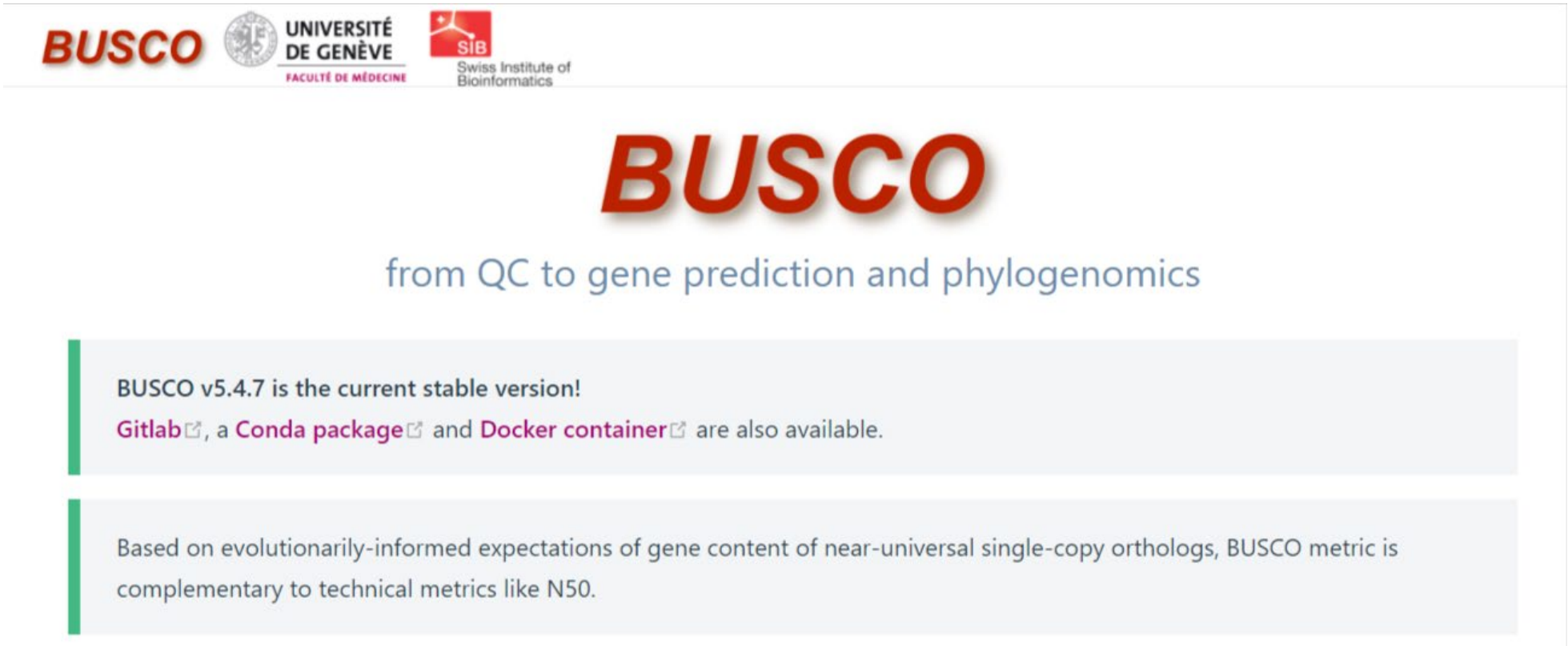
Installing software on an HPC system

1) Problems

- **Traditional Linux solution:**
  - Compiling from source code

1) Problems

a) Dependencies (Welcome to Linux!)



1) Problems

a) **Dependencies** (Welcome to Linux!)

Third-party components

A full installation of BUSCO requires *Python 3.3+* (2.7 is not supported from v4 onwards), *BioPython*, *pandas*, *BBMap*, *tBLASTn 2.2+*, *Augustus 3.2+*, *Prodigal*, *Metaeuk*, *HMMER3.1+*, *SEPP*, and *R + ggplot2* for the plotting companion script. Some of these tools are necessary only for analysing certain type of organisms and input data, or for specific run modes.

- https://biopython.org/
- https://pandas.pydata.org/
- https://jgi.doe.gov/data-and-tools/software-tools/bbtools/
- https://ftp.ncbi.nlm.nih.gov/blast/executables/blast+/LATEST
- http://bioinf.uni-greifswald.de/augustus/
- https://github.com/soedinglab/metaeuk
- https://github.com/hyattpd/Prodigal
- http://hmmer.org/
- https://github.com/smirarab/sepp/
- https://www.r-project.org/

> Please make sure that each software package listed above works INDEPENDENTLY of BUSCO before attempting to run any BUSCO assessments.

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- http://bioinf.uni-greifswald.de/augustus/
- https://github.com/soedinglab/metaeuk
- https://github.com/hyattpd/Prodigal
- http://hmmer.org/
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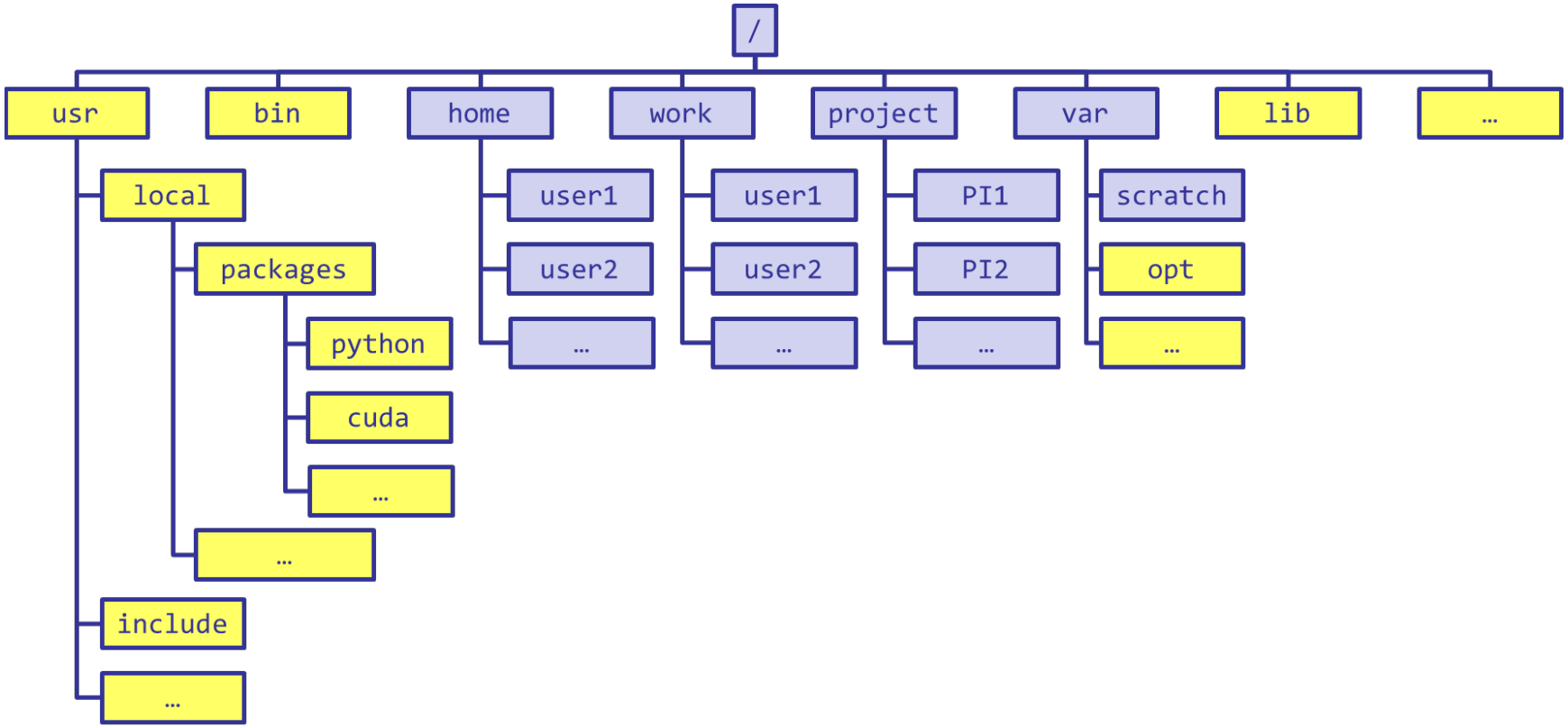
- Dependencies

The following dependencies are required for AUGUSTUS:

- for gzip compressed input: (set ZIPINPUT = false in common.mk if t… re not available)
  - libboost-iostreams-dev
  - zlib1g-dev
- for comparative AUGUSTUS (multi-species, CGP): (set COMPGENEPRED = false in co… raries required by the CGP version are not available. Augustus can then only be run in single-genome mode, which is what most users need.)
  - libgsl-dev
  - libboost-all-dev
  - libsuitesparse-dev
  - liblpsolve55-dev
  - libsqlite3-dev (add SQLITE = false to common.mk if this feature is not required or the required library is not available)
  - libmysql++-dev (add MYSQL = false to common.mk if this feature is not required or the required library is not available)
- for compiling utilities bam2hints and filterBam:
  - libbamtools-dev zlib1g-dev
- for compiling utility utrrnaseq:
  - libboost-all-dev (version must be >Boost_1_49_0)
- for compiling utility bam2wig:
  - Follow these instructions. Note that it shouldn't be a problem to compile AUGUSTUS without bam2wig. In practice, you can simply use `bamToWig.py` to accomplish the same task.
- For compiling homgenemapping (set BOOST = FALSE in auxprogs/homgenemapping/src/Makefile if the option --printHomologs is not required or the required libraries are not available)
  - libboost-all-dev
- for scripts:
  - Perl
  - Python3
- for the python3 script bamToWig.py:
  - twoBitInfo and faToTwoBit from http://hgdownload.soe.ucsc.edu/admin/exe . bamToWig.py will automatically download these tools to the working directory during execution if they are not in your $PATH.
  - SAMtools (available e.g. via package managers or here - see notes below)

1) Problems

b) Permission denied (Welcome to HPC!)



1) Problems

b) Permission denied (Welcome to HPC!)

```
[jasonli3@smic2 ~]$ module load python/3.6.2-anaconda-tensorflow
[jasonli3@smic2 ~]$ module li
Currently Loaded Modulefiles:
 1) python/3.6.2-anaconda-tensorflow
```

1) Problems

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Currently Loaded Modulefiles:
 1) python/3.6.2-anaconda-tensorflow
[jasonli3@smic2 ~]$ pip install geos
Collecting geos
  Downloading https://files.pythonhosted.org/packages/49/5b/b8acf74c01187a36aa41b6523deb9baa59c
    100% |                                | 409kB 3.0MB/s
```

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    100% |                                | 409kB 3.0MB/s
```

```
    os.makedirs(path)
  File "/usr/local/packages/python/3.6.2-anaconda/lib/python3.6/os.py", line 220, in makedirs
    mkdir(name, mode)
PermissionError: [Errno 13] Permission denied: '/usr/local/packages/python/3.6.2-anaconda/lib/p
You are using pip version 9.0.1, however version 23.0.1 is available.
You should consider upgrading via the 'pip install --upgrade pip' command.
[jasonli3@smic2 ~]$
```

1) Problems

b) Permission denied (Welcome to HPC!)

- If you ask Google / ChatGPT…

```
$ sudo yum install …

$ sudo apt-get install …

$ sudo make install
```

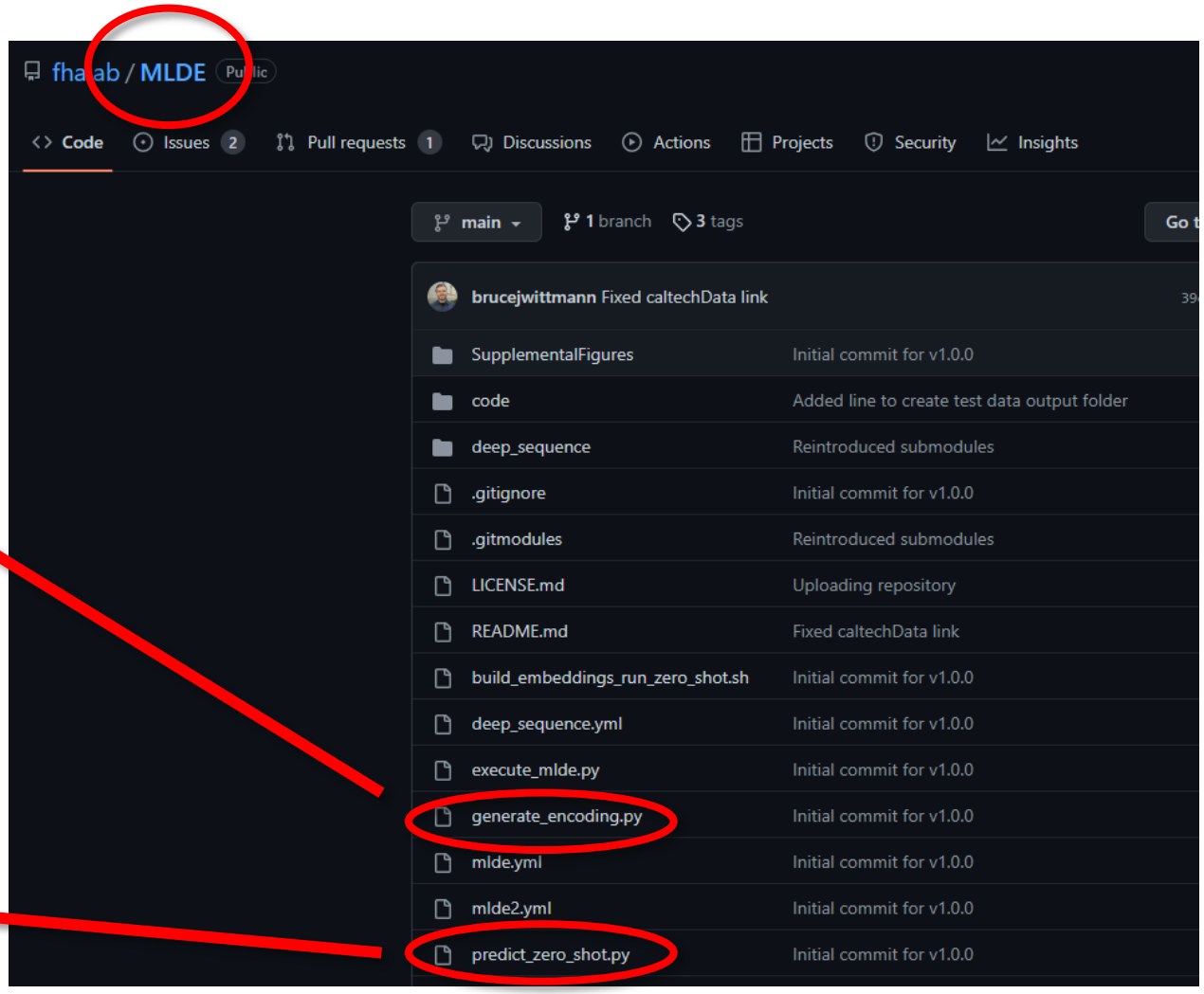
1) Problems

c) Conflicted packages

- What if I need two packages w/ conflicted dependencies?

Tensorflow 1.13

PyTorch > 1.5



d) Sharing / Migrating your environment

– Huge effort & large disk quota to install

- What if my colleagues want to use?
- What if I want to migrate a different cluster?

1) Problems

Any of those apply to you?

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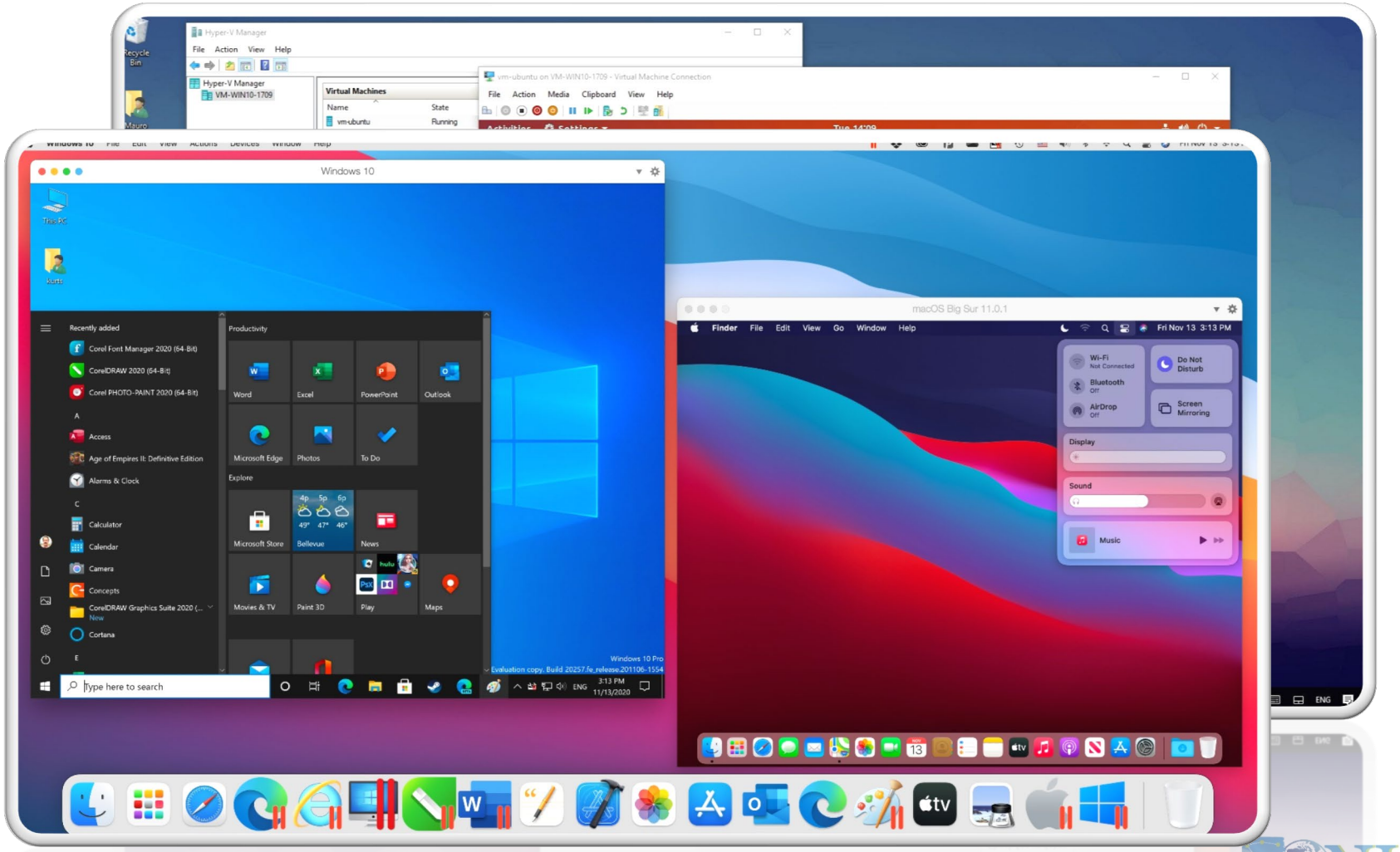
2) Container & Singularity

a) What is a container?

- **Virtual machine**
  - "Virtualize" / "mimic" an **entire computer** on another computer
  - Virtualize both **hardware** and **software**



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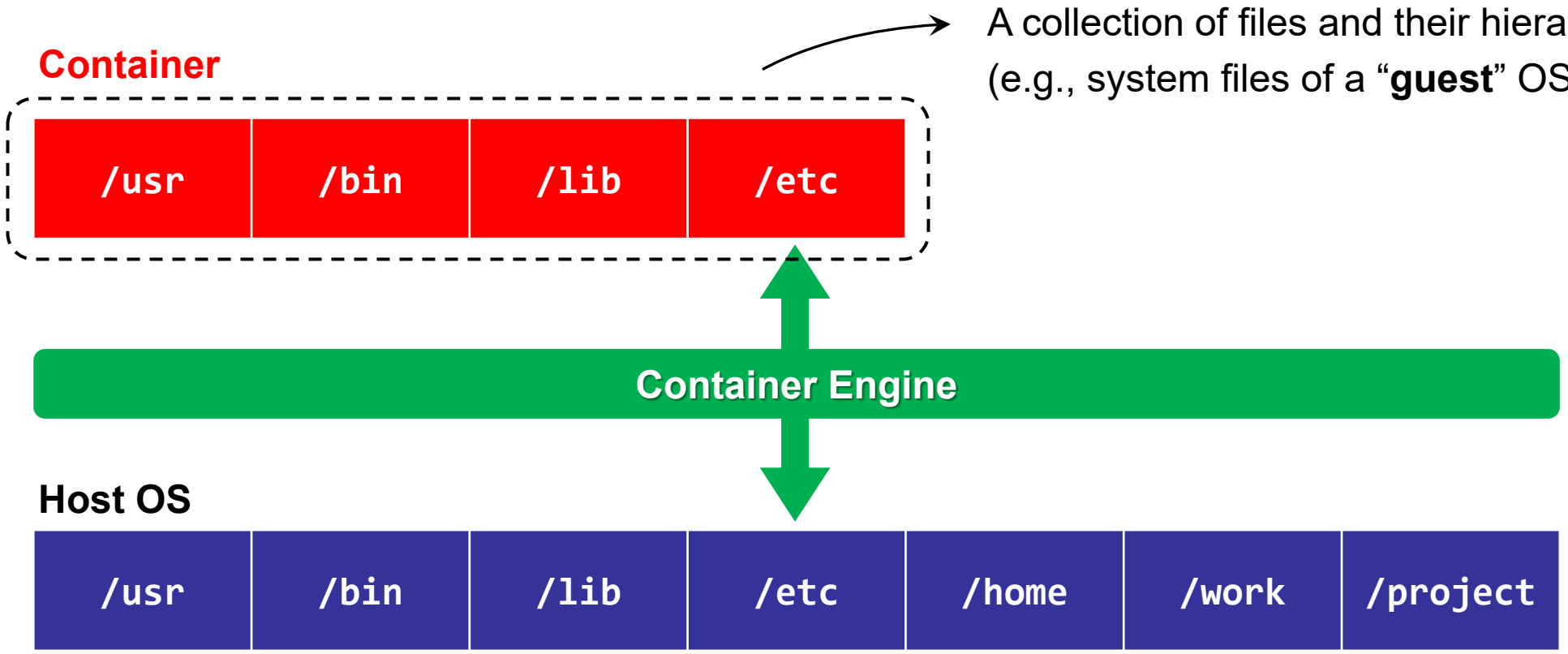
a) What is a container?

- **Container:**
  - A **lightweight** and **fast** virtual machine
  - Only virtualize the **Operation System** (meaning, does not virtualize hardware)
  - Only virtualize **Linux** on **Linux**

2) Container & Singularity

a) What is a container?



2) Container & Singularity

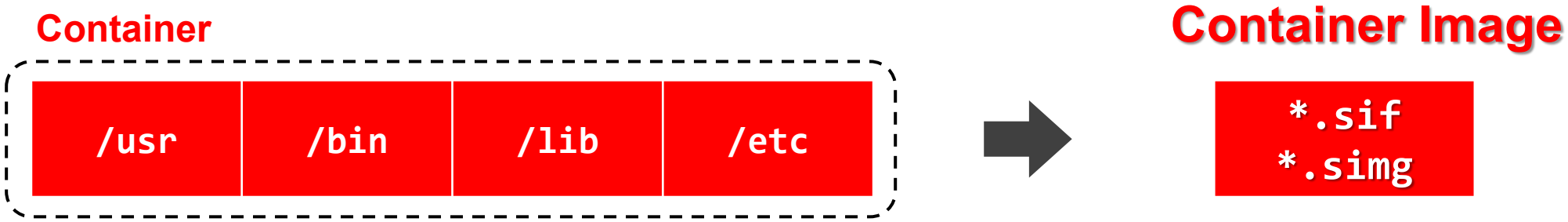
a) What is a container?

/usr	/bin	/lib	/etc	/home	/work	/project

- **A "chimera" system:**
  - Can virtualize **an entirely different OS** !
  - Can contain other **software packages** (inc. dependencies, environment settings, etc.) installed in the guest OS

2) Container & Singularity

a) What is a container?



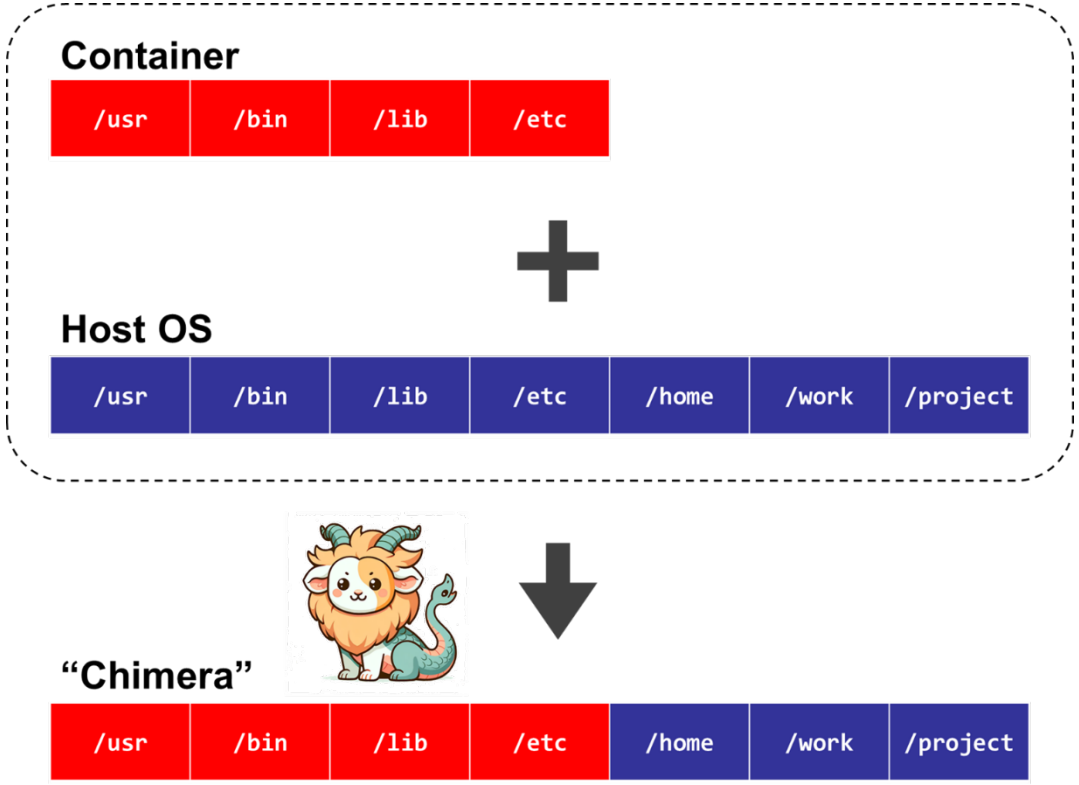
2) Container & Singularity

a) What is a container?

- **Properties:**
  - **Self-contained**

    All dependencies can be installed within the container
  - **Isolated**

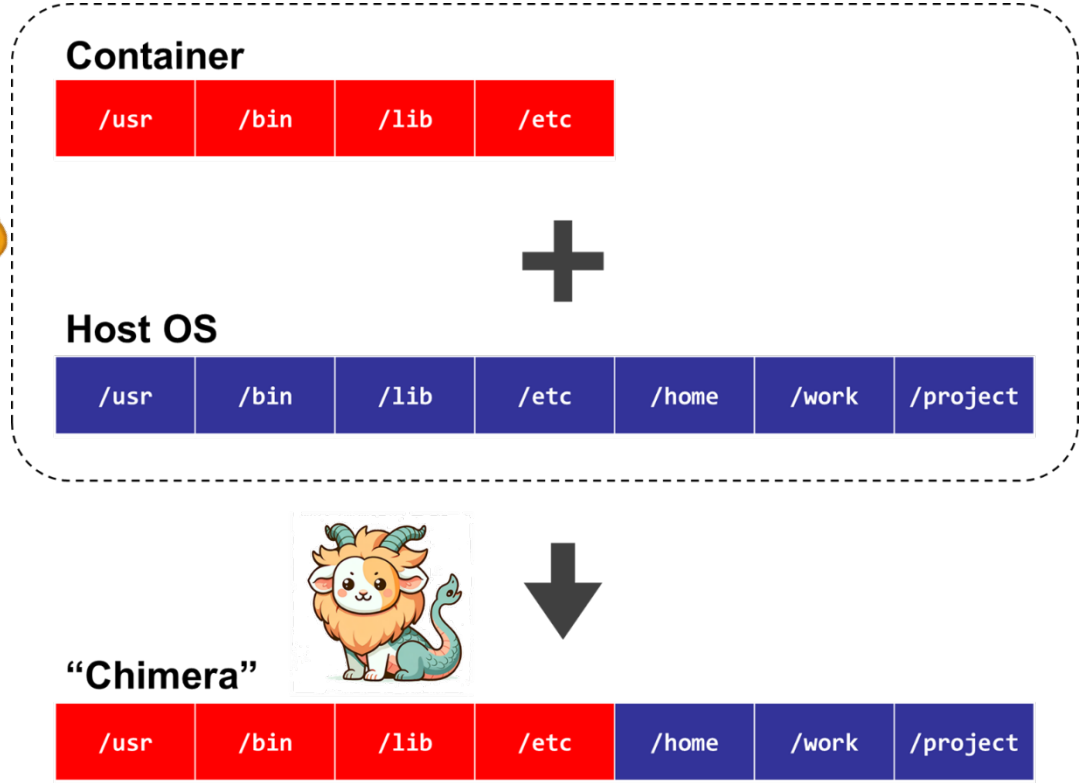
    Whatever happens in a container stays in that container…



b) How does it solve my problems?

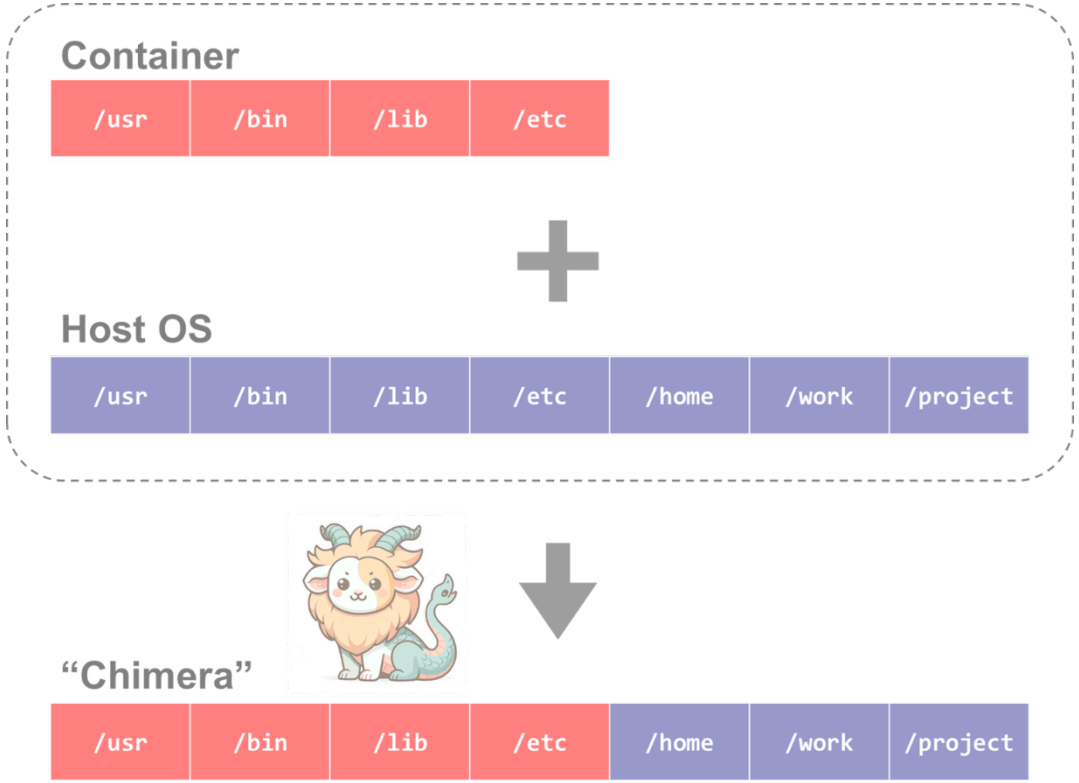
- **Dependency issue**
  - Pack all dependencies (even OS) in container
  - Can use `apt-get` or `yum`
  - **Developers now release containers!**

- **Permission issue**
  - Can't write to certain paths on HPC, but **CAN** write to them in container
- **Conflicted packages**
  - Install in different containers.
- **Share / Migrate**
  - Copy-paste a container image!



c) What is Singularity?

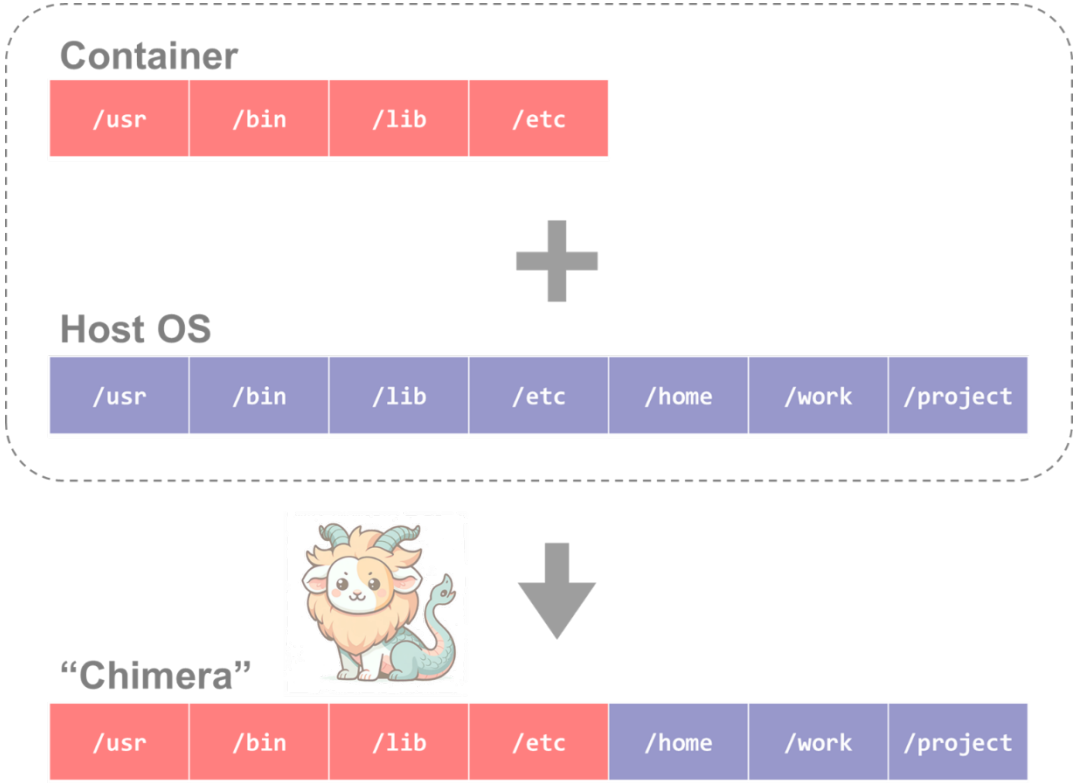
Technology →



c) What is Singularity?

Singularity

↑ **Software** system that implements the technology



c) What is Singularity?

c) What is Singularity?

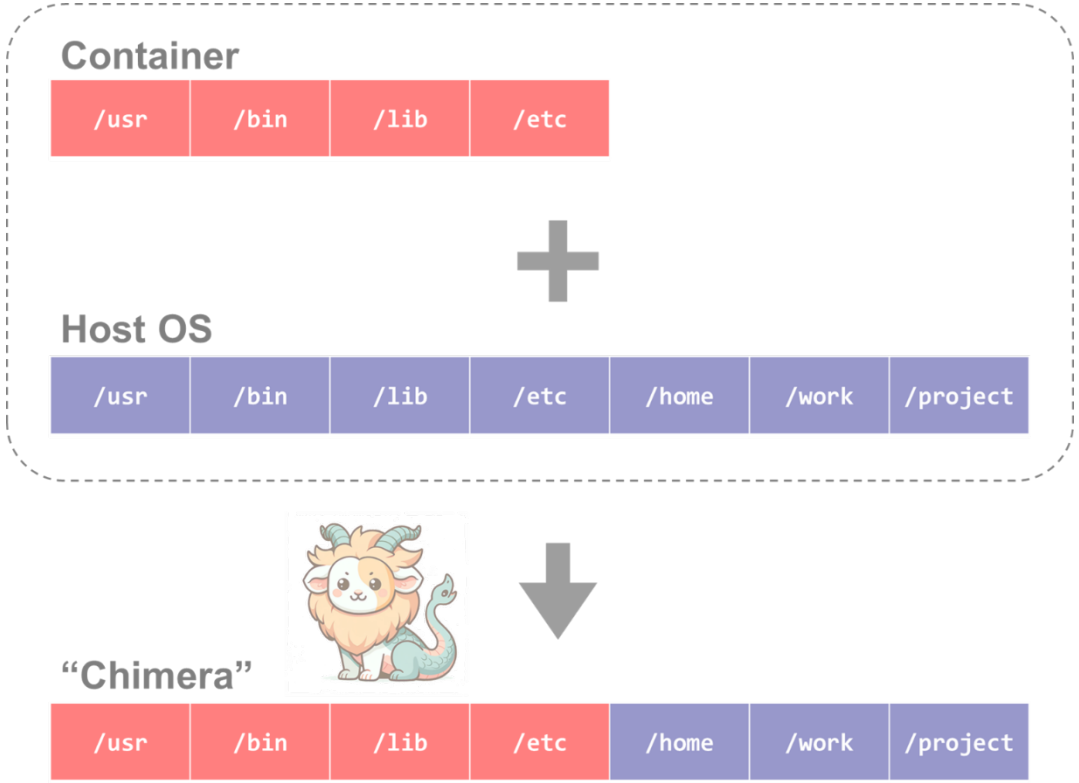
- Does **NOT** need root privileges
- "**Container for HPC**"

- **Needs** root privileges

Summary

Technology that helps with software installation →

↓ **Software** system that implements the technology



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1) What you need

- **Singularity availability**

  a) On **all clusters**
  - ✓ **LSU HPC**: SMIC, Deep Bayou, SuperMike 3
  - ✓ **LONI**: QB2, QB3

  b) Only on **computing nodes**
  - × Unavailable on head nodes
  - ✓ Must start a job (interactive & batch)

  c) To **all users**
  - × No additional action required

1) What you need

To …	What you need …
Run an Existing Container Image	• Access to our HPC systems - An active account - An active allocation

1) What you need

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2) Basic commands

- **Available images**

  – On all clusters: `/home/admin/singularity`

```
(base) [jasonli3@mike1 ~]$ ls /home/admin/singularity
abinit.v9.8.3.sif                   jax-0.4.13-gpu-jupyter.sif
alphafold-catgumag-2.2.sif          MuST-1.8.7.sif
bowtie2-2.5.1.sif                   openpose.sif
busco-5.4.7.sif                     pytorch-2.0.1-gpu-jupyter.sif
clara.400-1.sif                     rstudio-2023.03.1-446-rocky8.sif
deepmd-kit_2.0.3_cuda11.3_gpu.sif   salmon-1.10.2.sif
deepmd-kit_2.2.1_cuda11.6_gpu.sif   tensorflow-2.13.0-gpu-jupyter.sif
delft3dfm_r142632_05032023.sif      trinity-2.15.1.sif
delft3dfm_r142632.sif               ubuntu-training.sif
delft3d_r142586.sif
```

2) Basic commands

a) Common usage 1: Open a shell in the image

Syntax		Description
`singularity shell`	`<container>`	Starts a shell in the image

Try me: `/home/admin/singularity/ubuntu-training.sif`

2) Basic commands

a) Common usage 1: Open a shell in the image

Syntax		Description
`singularity shell [options] <container>`		Starts a shell in the image
`[Options]`	`-B /path/to/bind`	Bind a path(s) • /home is bound by default
	`--nv`	Enable Nvidia GPU

2) Basic commands

b) Common usage 2: Execute a single command in the image

Syntax	Description
`singularity exec <container> <command>`	Execute a command in the image

Try me: `/home/admin/singularity/ubuntu-training.sif`

2) Basic commands

b) Common usage 2: Execute a single command in the image

Syntax		Description
`singularity exec [options] <container> <command>`		Execute a command in the image
`[Options]`	`-B /path/to/bind`	Bind a path(s) • /home is bound by default
	`--nv`	Enable Nvidia GPU

c) Another (less) common usage: Run a prewritten script

Syntax		Description
`singularity run [options] <container>`		Run a prewritten script
`[Options]`	`-B /path/to/bind`	Bind a path(s) • /home is bound by default
	`--nv`	Enable Nvidia GPU

2) Basic commands

- **Quick recap**

Syntax	Description
`singularity shell [options] <container>`	Run a prewritten script
`singularity exec [options] <container> <command>`	Execute a command in the image
`singularity run [options] <container>`	Run a prewritten script

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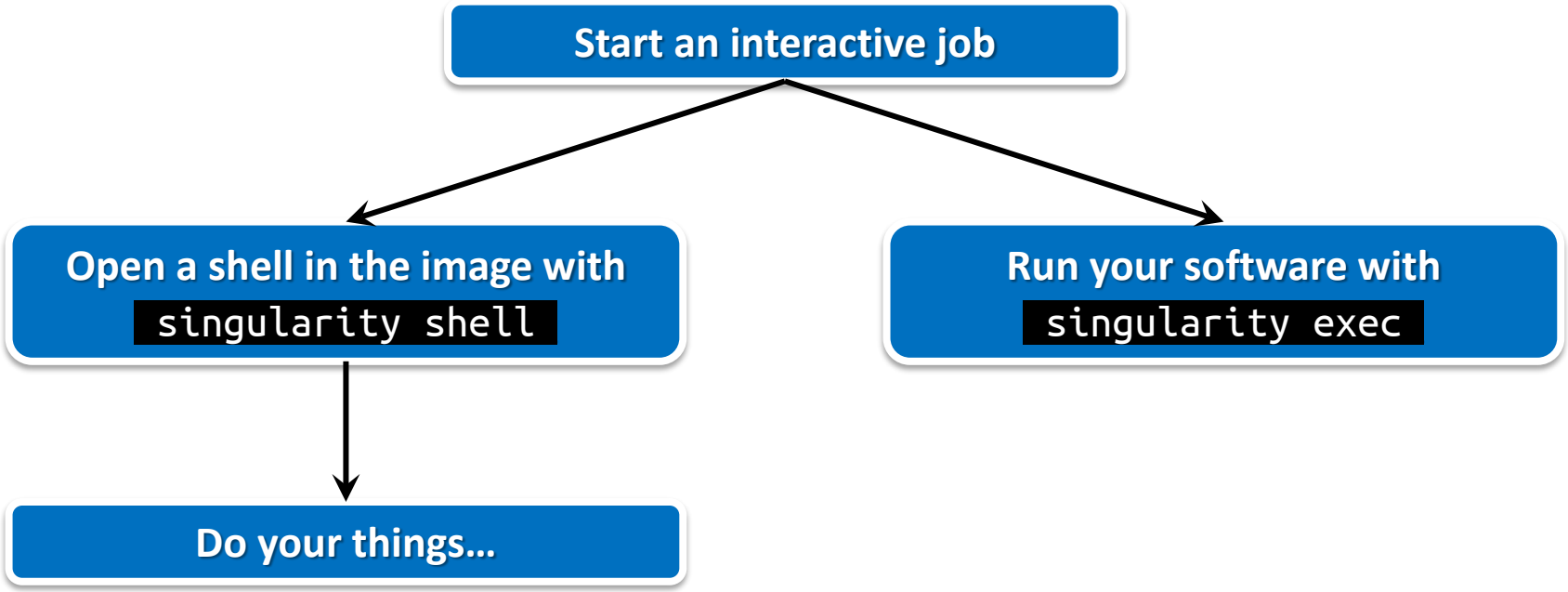
3) Run jobs with Singularity

- **Job types and commands**

Job Type	Commands	Purpose
Interactive	• `singularity shell [options] <container>` • `singularity exec [options] <container> <command>`	• Debugging & testing
Batch	• `singularity exec [options] <container> <command>`	• Production

3) Run jobs with Singularity

a) Interactive job



3) Run jobs with Singularity

b) Batch job

PBS

```
#!/bin/bash
#PBS -A <Allocation name>
#PBS -q workq
#PBS -l nodes=1:ppn=20
#PBS -l walltime=24:00:00


cd /to/work/directory
IMG=/home/admin/singularity/ubuntu-training.sif

singularity exec -B /work,/project $IMG \
  python myjob.py
```

Example

Slurm

```
#!/bin/bash
#SBATCH -A <Allocation name>
#SBATCH -p workq
#SBATCH -N 1
#SBATCH -n 64
#SBATCH -t 24:00:00

cd /to/work/directory
IMG=/home/admin/singularity/ubuntu-training.sif

singularity exec -B /work,/project $IMG \
  python myjob.py
```

Example

Summary

Summary

Syntax	Description
`singularity shell [options] <container>`	Run a prewritten script
`singularity exec [options] <container> <command>`	Execute a command in the image
`singularity run [options] <container>`	Run a prewritten script

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alphafold-catgumag-2.2.sif          MuST-1.8.7.sif
bowtie2-2.5.1.sif                   openpose.sif
busco-5.4.7.sif                     pytorch-2.0.1-gpu-jupyter.sif
clara.400-1.sif                     rstudio-2023.03.1-446-rocky8.sif
deepmd-kit_2.0.3_cuda11.3_gpu.sif   salmon-1.10.2.sif
deepmd-kit_2.2.1_cuda11.6_gpu.sif   tensorflow-2.13.0-gpu-jupyter.sif
delft3dfm_r142632_05032023.sif      trinity-2.15.1.sif
delft3dfm_r142632.sif               ubuntu-training.sif
delft3d_r142586.sif
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1) What you need

```
(base) [jasonli3@mike4 ~]$ ll /home/admin/singularity
total 78269032
-rwxr-xr-x 1 root singularity  4555411456 Jun  7 20:27 abinit.v9.8.3.sif
-rwxr-xr-x 1 root singularity  3167338496 Oct  3  2022 alphafold-catgumag-2.2.sif
-rwxr-xr-x 1 root singularity   118206464 Sep 11 11:00 bowtie2-2.5.1.sif
-rwxr-xr-x 1 root singularity   822177792 Aug 22 09:00 busco-5.4.7.sif
-rwxr-xr-x 1 root singularity  2155438080 Nov  9  2022 clara.400-1.sif
-rwxr-xr-x 1 root singularity  3285417984 Jun  6 13:13 deepmd-kit_2.0.3_cuda11.3_gpu.sif
-rwxr-xr-x 1 root singularity  3390902272 Jun  5 20:34 deepmd-kit_2.2.1_cuda11.6_gpu.sif
-rwxr-xr-x 1 root singularity  9305526272 May  3 12:56 delft3dfm_r142632_05032023.sif
-rwxr-xr-x 1 root singularity 11812220928 Jun 27 23:50 delft3dfm_r142632.sif
-rwxr-xr-x 1 root singularity 11594326016 Jul 26 00:05 delft3d_r142586.sif
-rwxr-xr-x 1 root singularity  5152387072 Sep 15 23:52 jax-0.4.13-gpu-jupyter.sif
-rwxr-xr-x 1 root singularity  7603736576 Jul 20 14:57 MuST-1.8.7.sif
-rwxr-xr-x 1 root singularity  5322223616 Jun 20 14:26 openpose.sif
-rwxr-xr-x 1 root singularity  4016316416 Aug  7 23:56 pytorch-2.0.1-gpu-jupyter.sif
-rwxr-xr-x 1 root singularity   911499264 May 25 09:48 rstudio-2023.03.1-446-rocky8.sif
-rwxr-xr-x 1 root singularity    42639360 Sep 21 12:22 salmon-1.10.2.sif
-rwxr-xr-x 1 root singularity  4079706112 Aug  8 00:32 tensorflow-2.13.0-gpu-jupyter.sif
-rwxr-xr-x 1 root singularity  2739630080 Aug 30 19:40 trinity-2.15.1.sif
-rwxr-xr-x 1 root singularity    71102464 Sep  7 11:50 ubuntu-training.sif
```

1) What you need

```
(base) [jasonli3@mike4 ~]$ ll /home/admin/singularity
total 78269032
-rwxr-xr-x 1 root singularity  4555411456 Jun  7 20:27 abinit.v9.8.3.sif
-rwxr-xr-x 1 root singularity  3167338496 Oct  3  2022 alphafold-catgumag-2.2.sif
-rwxr-xr-x 1 root singularity   118206464 Sep 11 11:00 bowtie2-2.5.1.sif
-rwxr-xr-x 1 root singularity   822177792 Aug 22 09:00 busco-5.4.7.sif
-rwxr-xr-x 1 root singularity  2155438080 Nov  9  2022 clara.400-1.sif
-rwxr-xr-x 1 root singularity  3285417984
-rwxr-xr-x 1 root singularity  3390902271
-rwxr-xr-x 1 root singularity  9305526271
-rwxr-xr-x 1 root singularity 11812220928
-rwxr-xr-x 1 root singularity 11594326016
-rwxr-xr-x 1 root singularity  5152387071
-rwxr-xr-x 1 root singularity  7603736576
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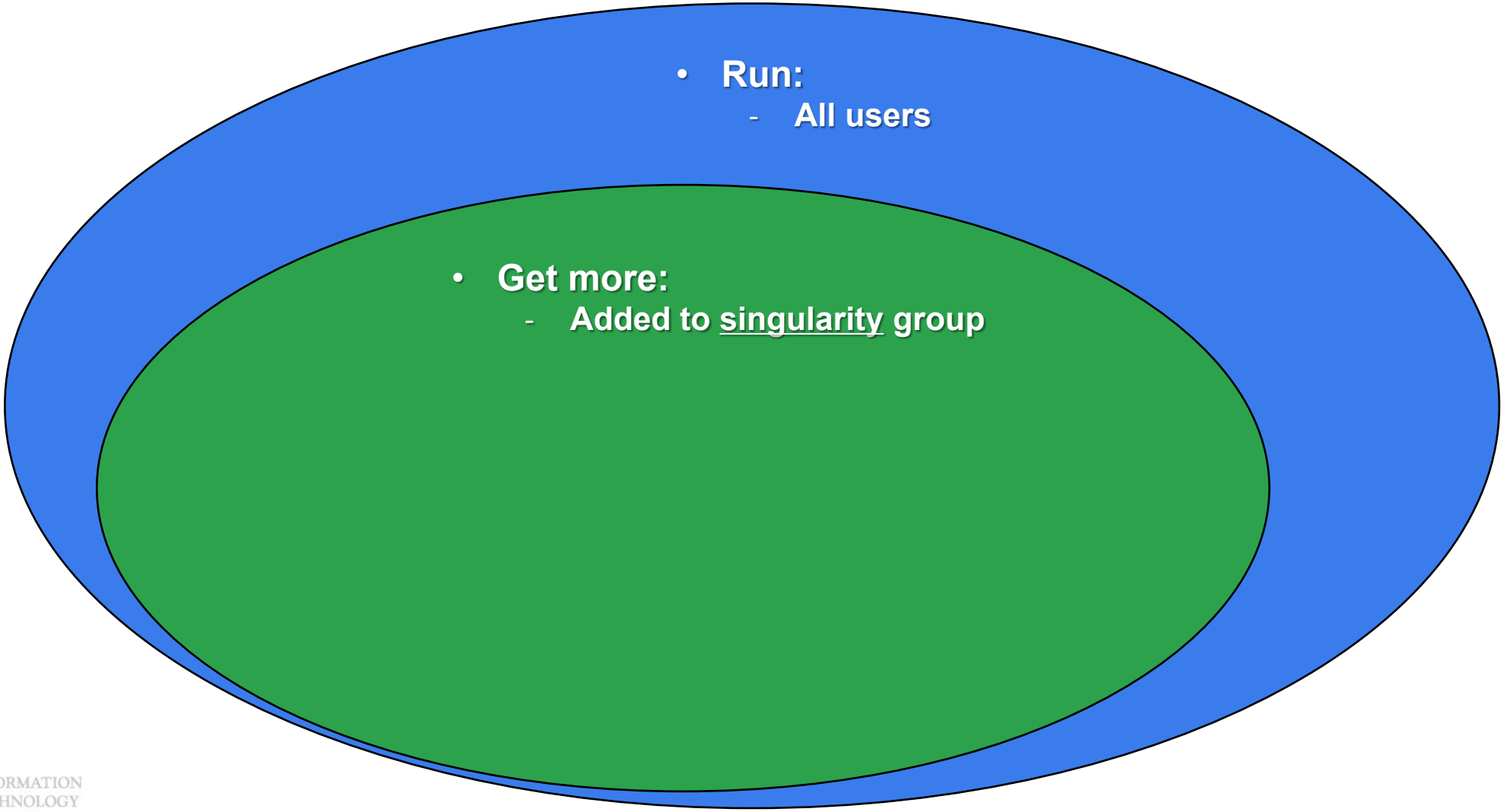
-rwxr-xr-x 1 root singularity    71102464 Sep  7 11:50 ubuntu-training.sif
```

Singularity images must belong to "**singularity**" group to run on our clusters!

1) What you need

To …	What you need …
Run an Existing Container Image	• Access to our HPC systems - An active account - An active allocation
Get More Container Images	• (Everything above) • Added to **Singularity** group - Needed to change **group ownership** - Send email to sys-help@loni.org to request

1) What you need



Outlines

1. Why Container?
   1) Problems
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2. Run an Existing Container Image
   1) What you need
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   3) Running jobs with Singularity
3. **Get More Container Images**
   1) What you need
   2) Where to get
   3) How to get
4. Build Your Own Container Image
   1) What you need
   2) Typical workflow
   3) Make it easier - Recipe

2) Where to get

- **You can get container images from a lot of places**
  - ➢ **Not that you should!**
- **Concerns?**
  - **Reliability** (some third-party or untested images may not work)
  - **Security risk** (some untrustworthy publishers may pack something you don't know about)
- **Solution**
  - Always get from a source that **you can trust**

2) Where to get

- **Tier 1: Developer release (official release)**
  - On software's official website, look for "**Docker**" / "**Singularity**" / "**Container**" / etc.
  - E.g., Tensorflow, Trinity, Salmon
- **Tier 2: Trustworthy third party**

Name	Notes
Biocontainers	• https://biocontainers-edu.readthedocs.io/en/latest/ • For biology
Nvidia NGC	• https://catalog.ngc.nvidia.com/containers • For Nvidia GPU
Bitnami	• https://bitnami.com/stacks/containers • By VmWare
Docker Hub **Quay.io**	• https://hub.docker.com/ & https://quay.io/ • Don't just trust everything you see there! • Look for Docker Official Image or Verified Publisher • Avoid third-party publishers that you don't know

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3) How to get

- **Steps:**

  a) Step 1: Pull the image

  b) Step 2: Change group ownership

3) How to get

a) Step 1: Pull the image

Syntax		Description
`singularity pull <source>`		Pull an image from source

`<source>`	`docker://container[:tag]`
	• (Compare to Docker command)
	`docker pull container[:tag]`
		Pull a Docker container and convert to Singularity
		• Many software's official container release is in Docker form (may or may not on Docker Hub)

	`http://www.myexample.com/container_image.sif`	Download an image file from a web source

3) How to get

a) Step 1: Pull the image

Syntax		Description
`singularity build <target> <source>`		Build an image from source (Advanced)
`<source>`	`docker://container[:tag]`	Build from a Docker container
	`container_image.sif`	Build from a local image file
	`container_sandbox/`	Build from a local **sandbox** (A directory form of a container)
	`container_recipe.def`	Build from a **recipe** (an instruction script of how to build an image)

3) How to get

a) Step 1: Pull the image

Syntax	Description
`singularity pull [options] [target] <source>`	Simple pull
`singularity build [options] <target> <source>`	Advanced build command

3) How to get

b) Step 2: Change group ownership

– What if you do not?

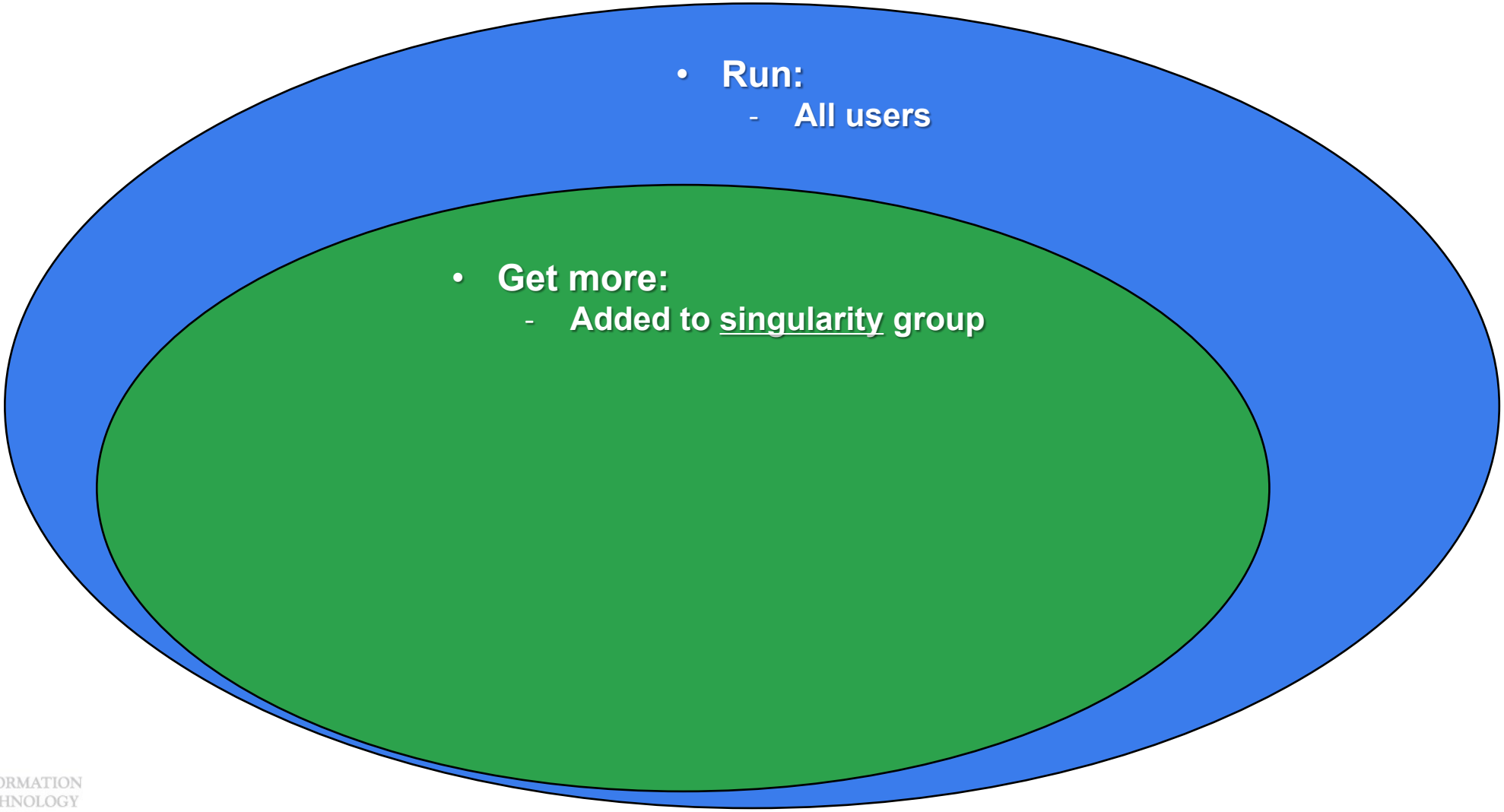
```
FATAL:   singularity image is not owned by required group(s)
```

– To solve it, run this:

```
$ chgrp singularity <container>
```

* You must be added to singularity group to finish this step

Summary



Summary

- **Steps:**

a) Step 1: Pull the image

Syntax	Description
`singularity pull [options] [target] <source>`	Simple pull
`singularity build [options] <target> <source>`	Advanced build command

b) Step 2: Change group ownership

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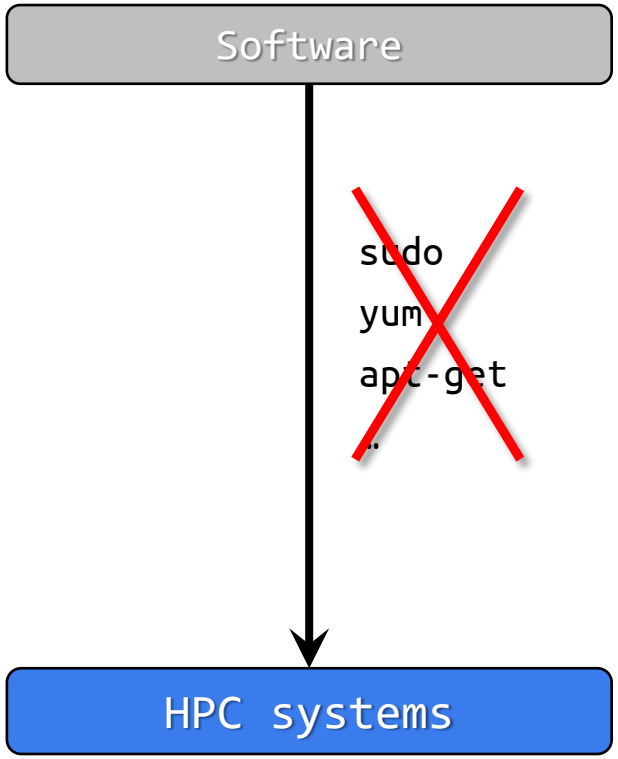
4. Build Your Own Container Image

- **Scenarios:**
  - I did not find any container release. Need to DIY.
  - Installation can be easily done using `sudo apt` or `sudo yum` if I have the permission.
  - I found a container, but need to make changes (e.g., adding something else).

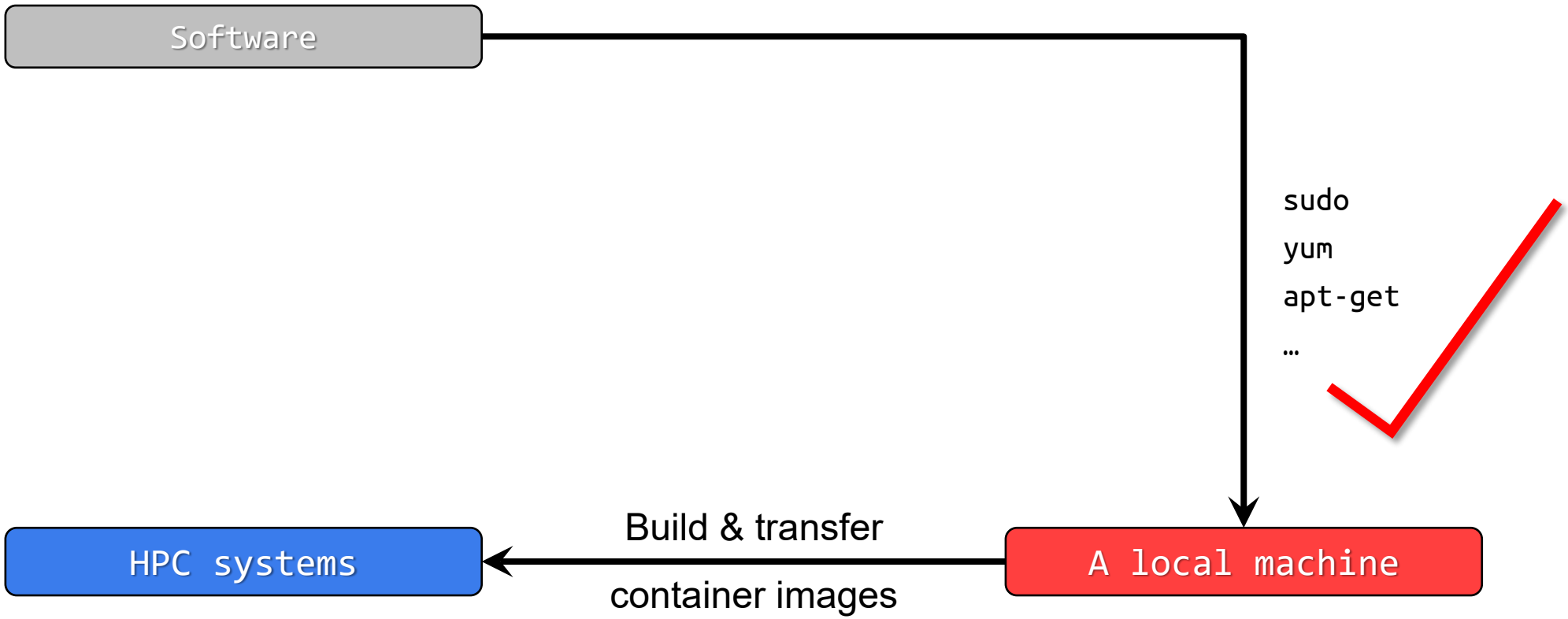
4. Build Your Own Container Image

- **Idea**



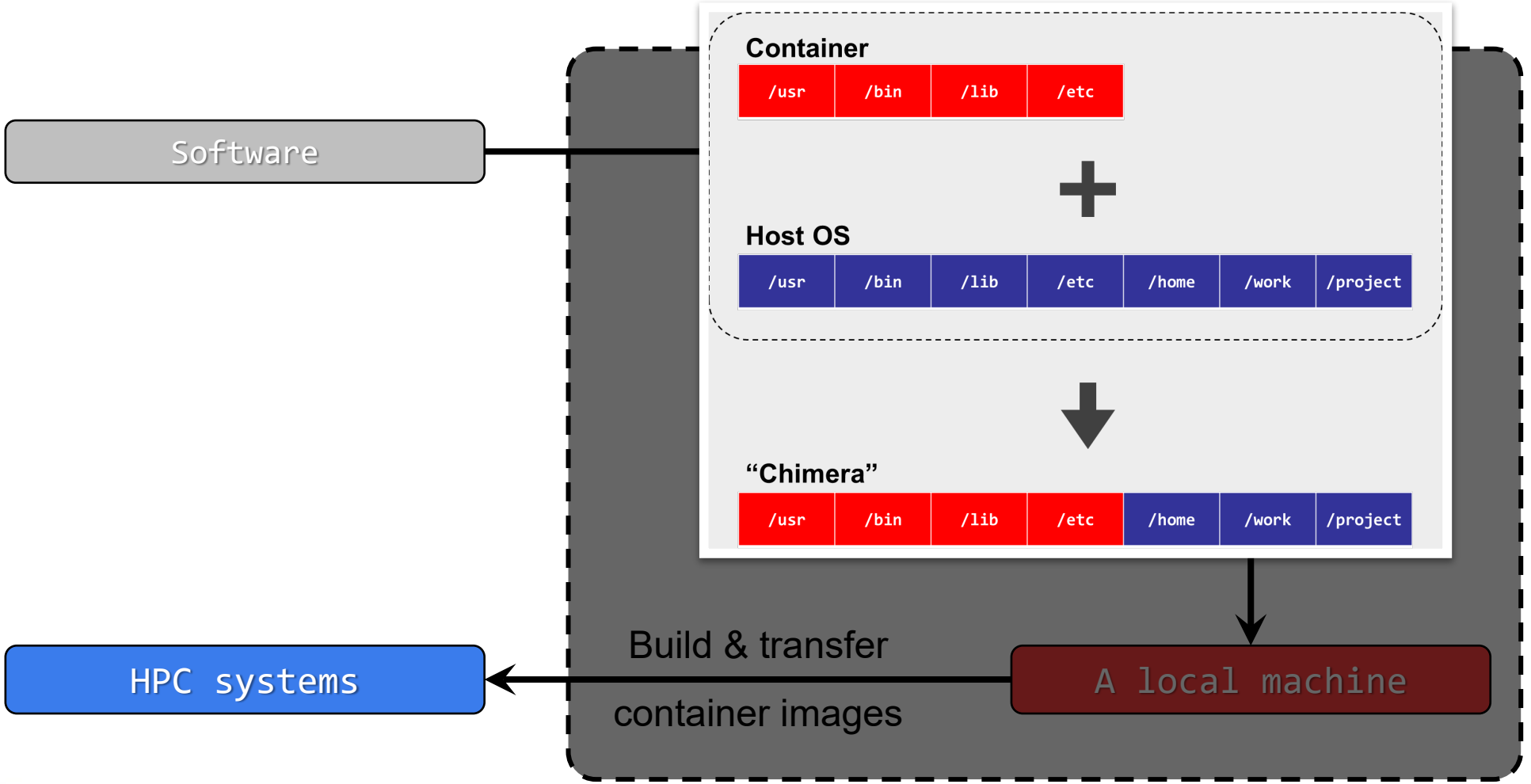
4. Build Your Own Container Image

- **Idea**



4. Build Your Own Container Image

- **Idea**



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1) What you need

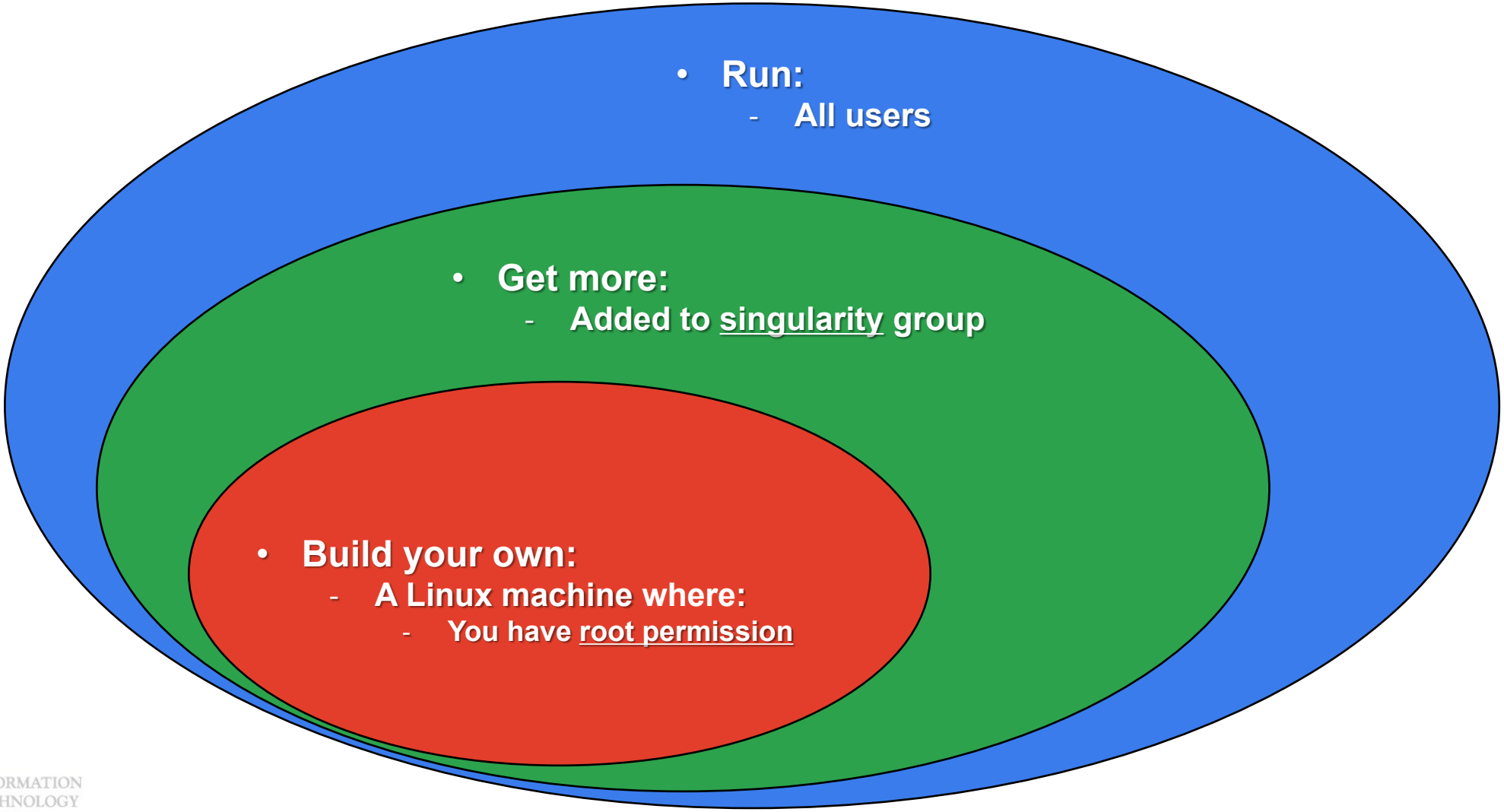
To …	What you need …

Run an Existing Container Image	• Access to our HPC systems
	  - An active account
	  - An active allocation

Get More Container Images	• (Everything above)
	• Added to **Singularity** group
	  - Needed to change **group ownership**
	  - Send email to sys-help@loni.org to request

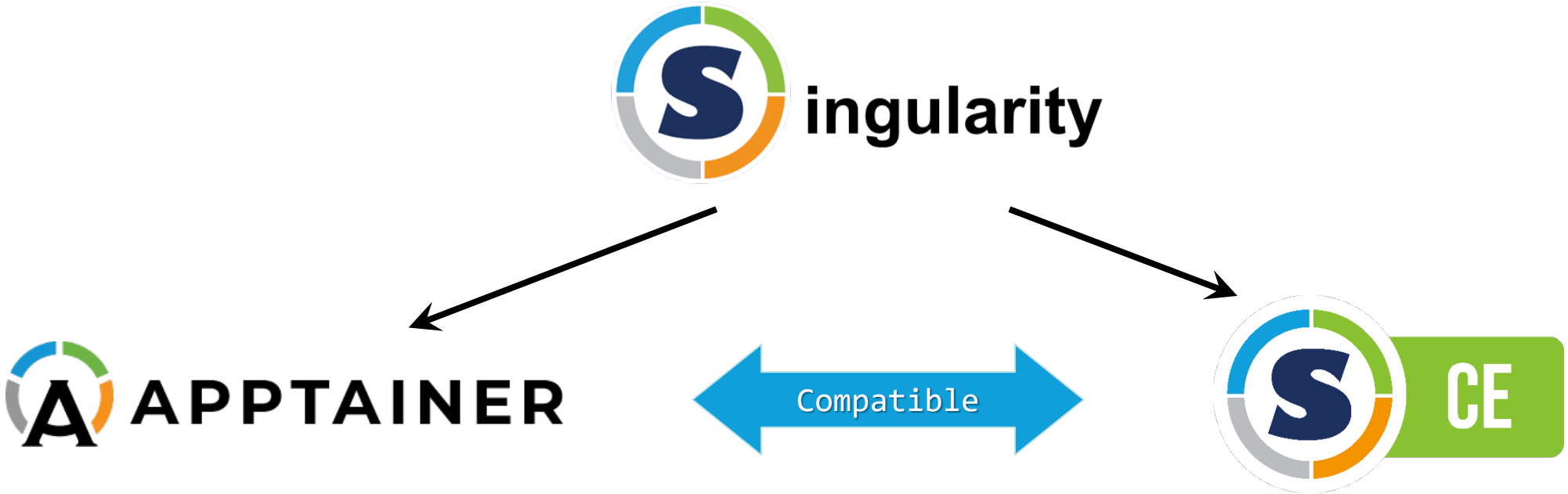
Build Your Own Container Image	• (Everything above) • A local Linux machine, where: - You have **root permission**

1) What you need



1) What you need

- **Install Singularity**



- Joined Linux Foundation
- Easier installation

- Community supported
- Installed on our clusters

[1] https://apptainer.org/docs/admin/main/installation.html
[2] https://docs.sylabs.io/guides/3.8/admin-guide/installation.html

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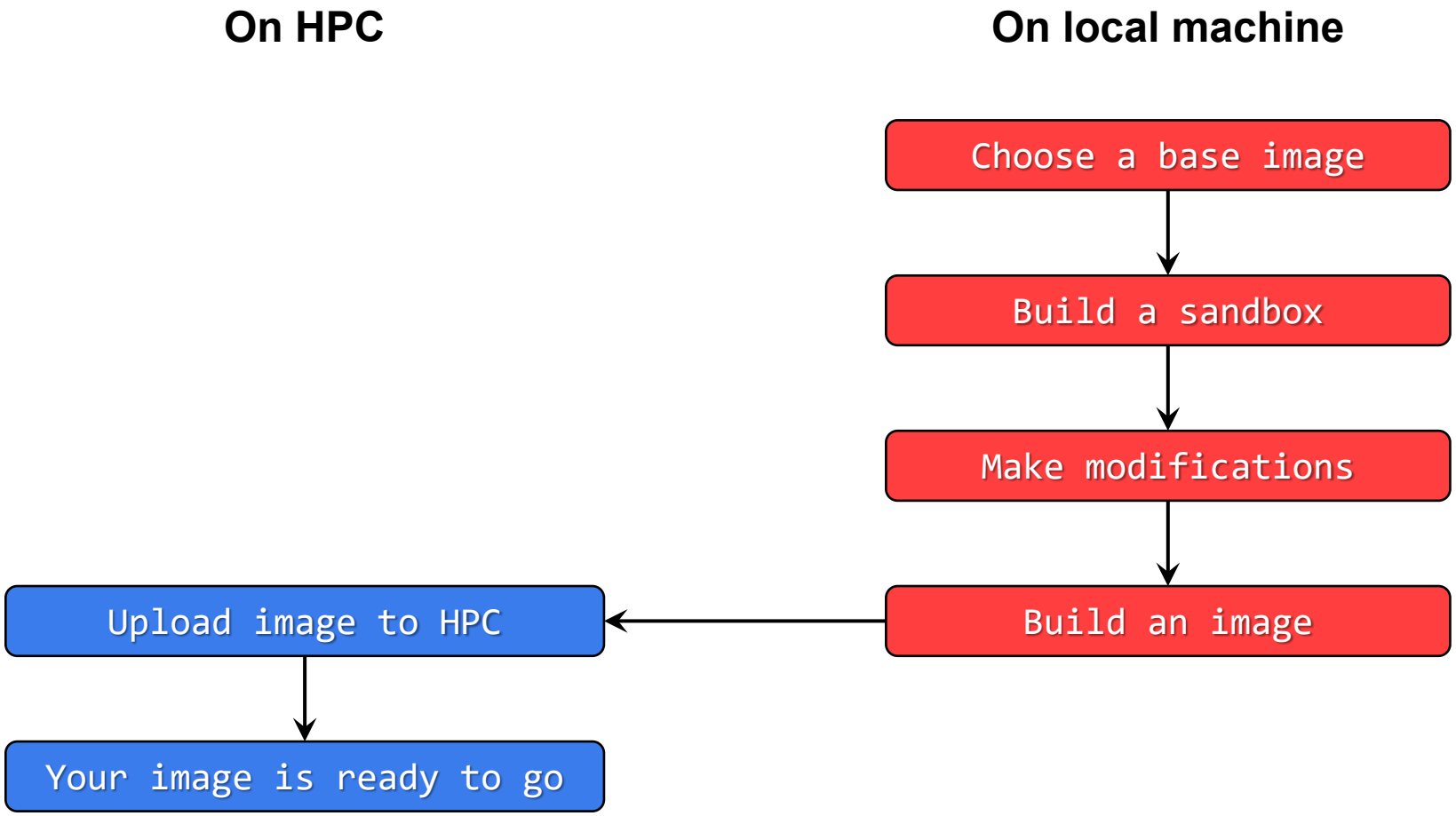
2) Typical workflow



2) Typical workflow

a) Choose a base image

Common choices	Typical scenarios
A minimum, "mint" OS (e.g., Ubuntu, Rocky, Debian, …)	• You cannot find an existing image with the software you need, and need to install from the scratch. • You need to build a minimum size image
A container with software already installed (e.g., TensorFlow, PyTorch, …)	• You need to modify an existing working image (e.g., add a Python module to Tensorflow image)

b) Build a sandbox

– What's a **sandbox** ?

- A **directory** form (unlike a single image file) of a container
- Allows modification

2) Typical workflow

b) Build a sandbox

```
$ singularity build [options] <target> <source>
```

<source>	docker://container[:tag]	Build from a Docker container
	container_image.sif	Build from a local image file
	container_sandbox/	Build from a local **sandbox** (A directory form of a container)
	container_recipe.def	Build from a **recipe** (an instruction script of how to build an image)

2) Typical workflow

b) Build a sandbox

```
$ singularity build --sandbox [options] <target> <source>
```

<source>	docker://container[:tag]	Build from a Docker container
	container_image.sif	Build from a local image file
	container_sandbox/	Build from a local **sandbox** (A directory form of a container)
	container_recipe.def	Build from a **recipe** (an instruction script of how to build an image)

2) Typical workflow

c) Make modifications

```
$ singularity shell [options] <container>
```

2) Typical workflow

c) Make modifications

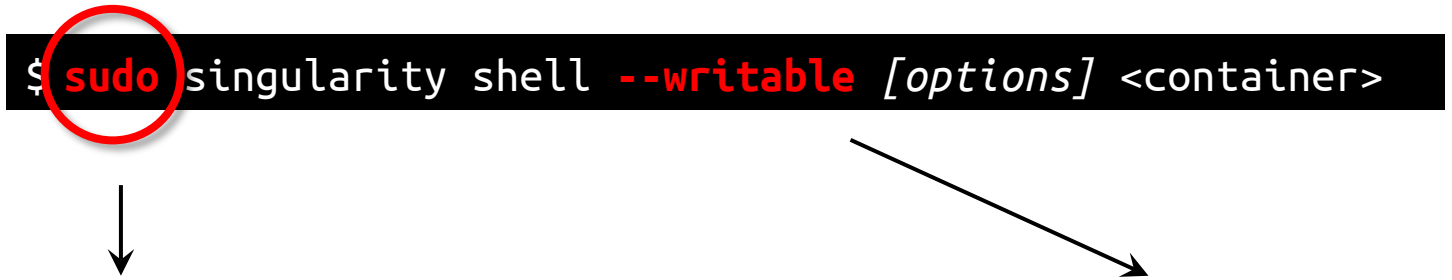
```
$ singularity shell --writable [options] <container>
```

i. Allows **writing** to the sandbox

   – Without it, just like running a regular container image

2) Typical workflow

c) Make modifications



ii. Run the container as **root**

- Grants root privilege in container
- Needed in most cases
- Technically not required, but cannot run things like `sudo apt` or `sudo yum` without it

i. Allows **writing** to the sandbox

- Without it, just like running a regular container image

2) Typical workflow

c) Make modifications

```
$ sudo singularity shell --writable [options] <container>
Singularity>
Singularity> apt update
Singularity> apt install ...
```

2) Typical workflow

d) Build an image from sandbox

```
$ singularity build [options] <target> <source>
```

<source>	docker://container[:tag]	Build from a Docker container
	container_image.sif	Build from a local image file
	container_sandbox/	Build from a local **sandbox** (A directory form of a container)
	container_recipe.def	Build from a **recipe** (an instruction script of how to build an image)

2) Typical workflow

d) Build an image from sandbox

```
$ sudo singularity build [options] <target> <source>
```

Modify with “**sudo**”? Build with “**sudo**”!

2) Typical workflow

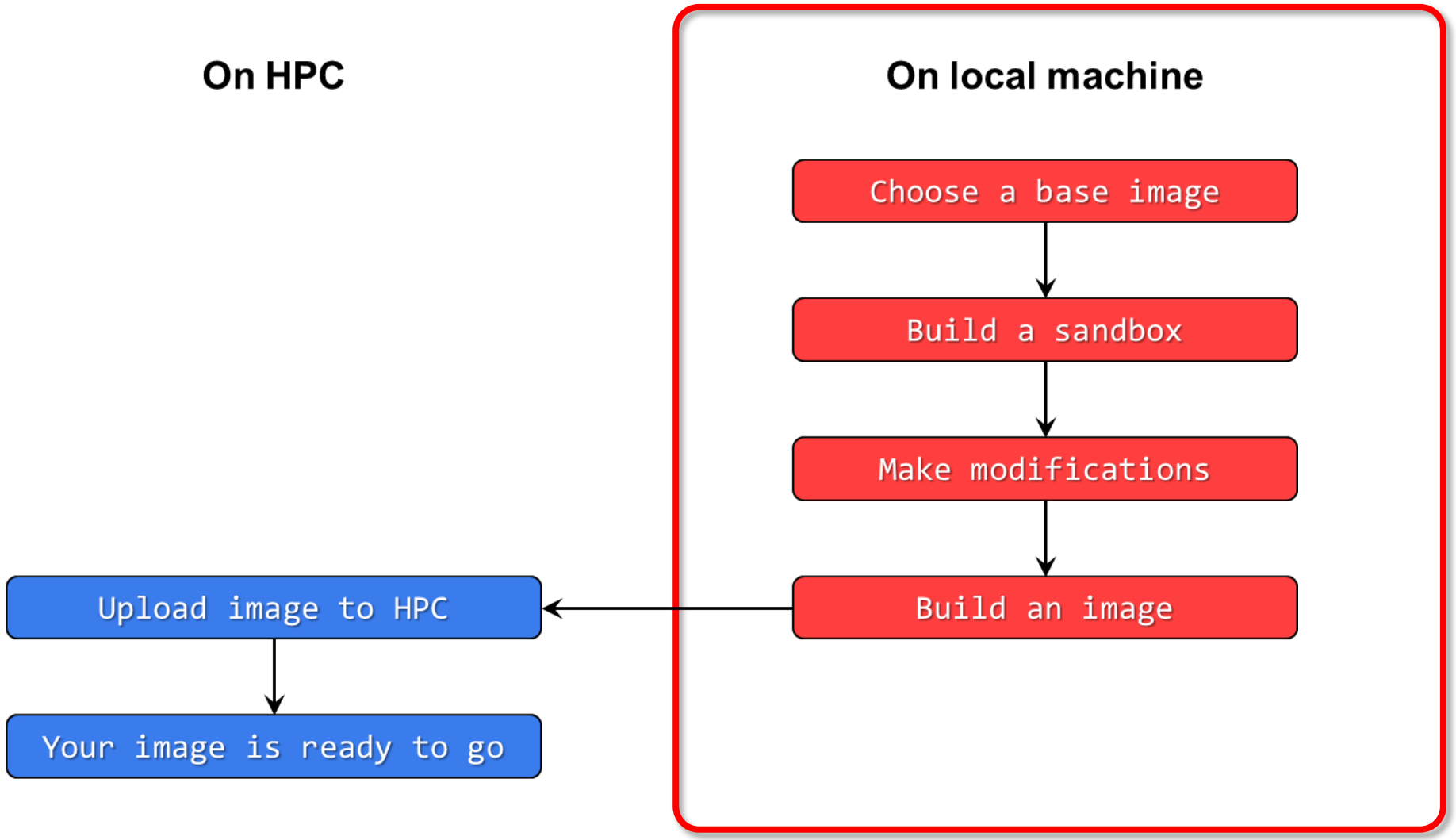
- **Quick recap**

To …	You need to …
Build a sandbox	`$ singularity build --sandbox ...`
Modify a sandbox	`$ sudo singularity shell --writable ...`
Build an image from sandbox	`$ sudo singularity build ...`

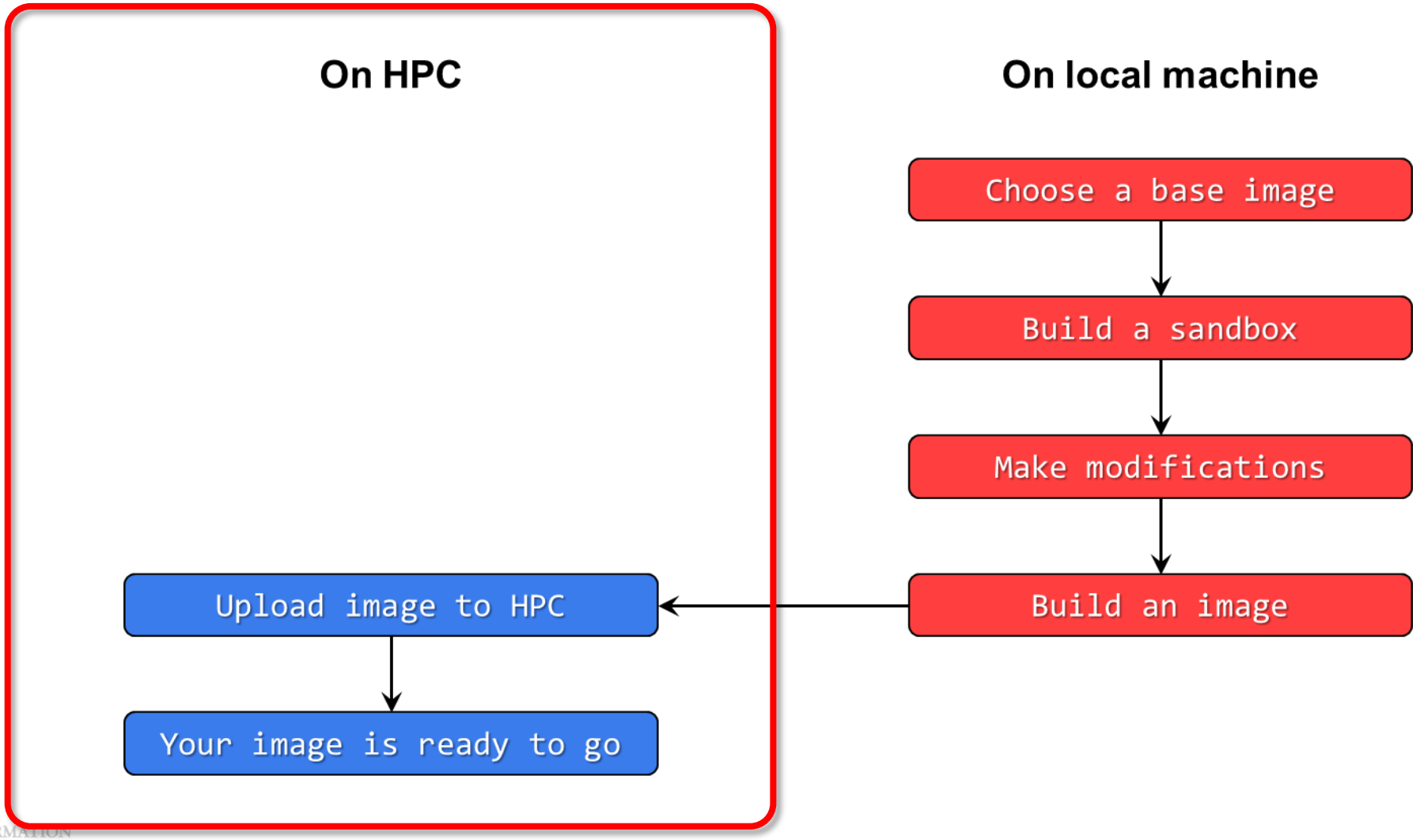
e) Upload image to HPC and run

Now! The moment of truth!

2) Typical workflow



2) Typical workflow



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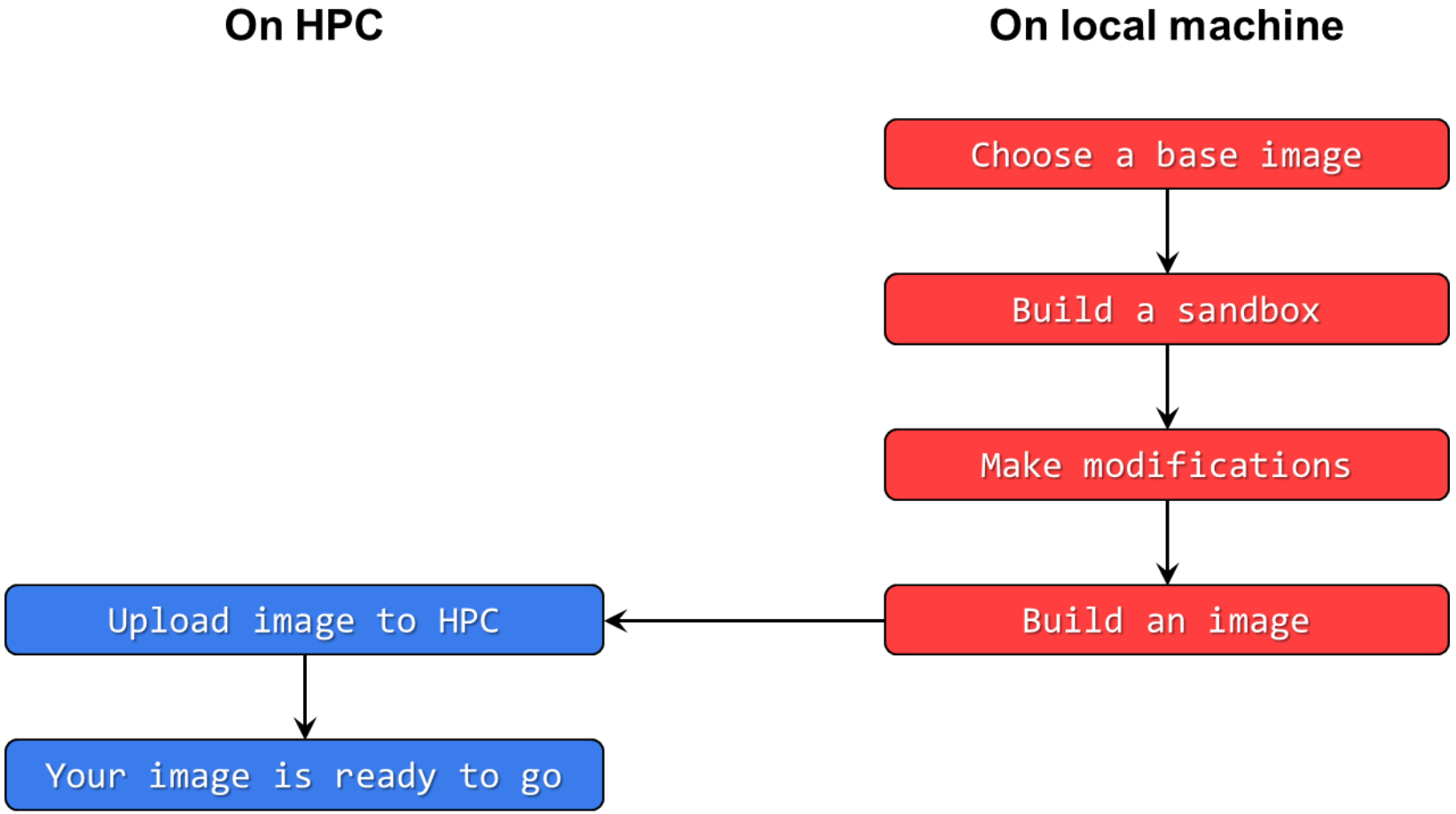
3) Make it easier - Recipe

- **Why?**



3) Make it easier - Recipe

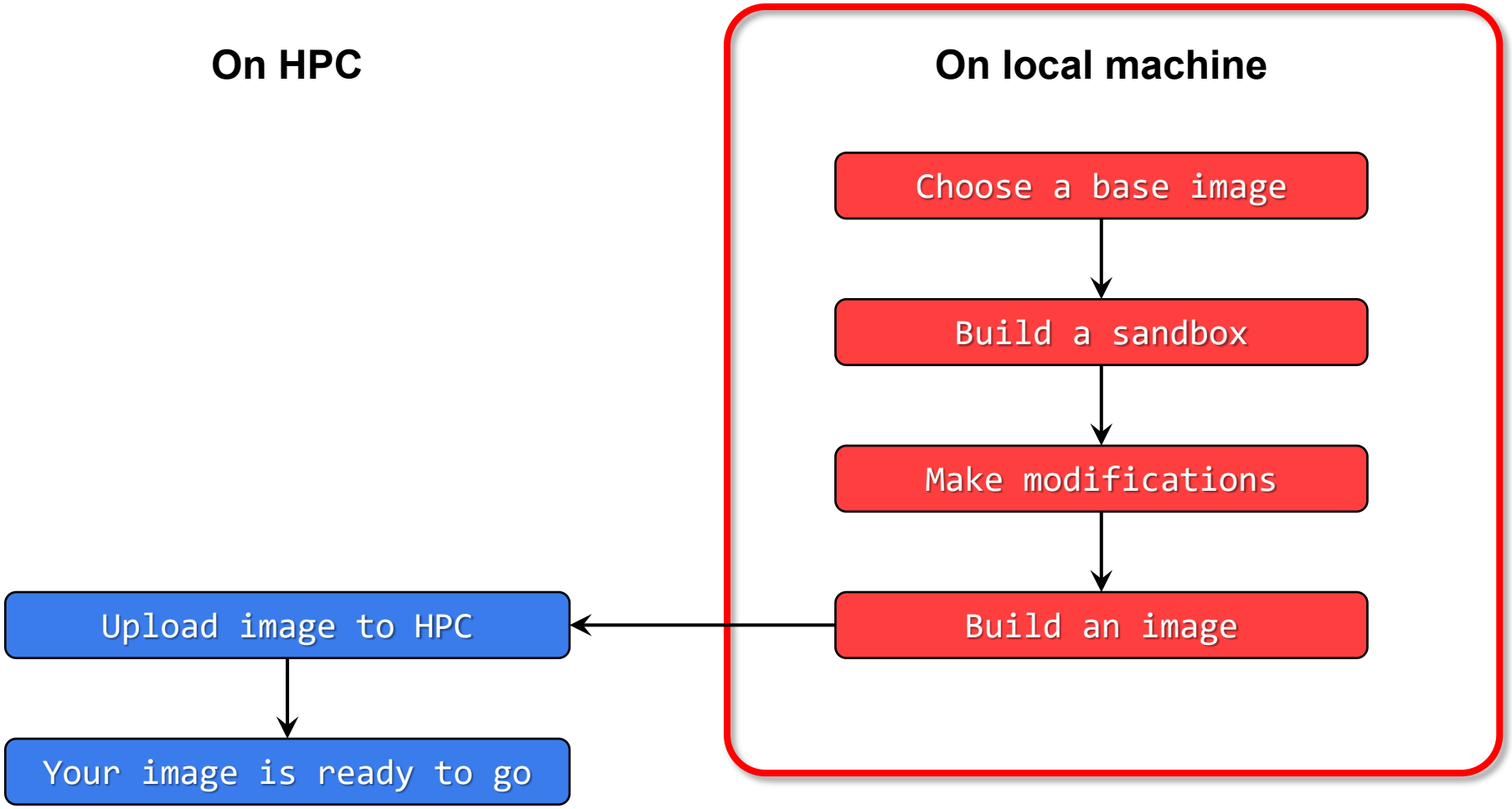
- **Why?**

Pros	Cons
• Flexibility	• Repeatability • Minimizing image size

- **Solution:**
  - **Recipe**: A text file containing instructions to build a container

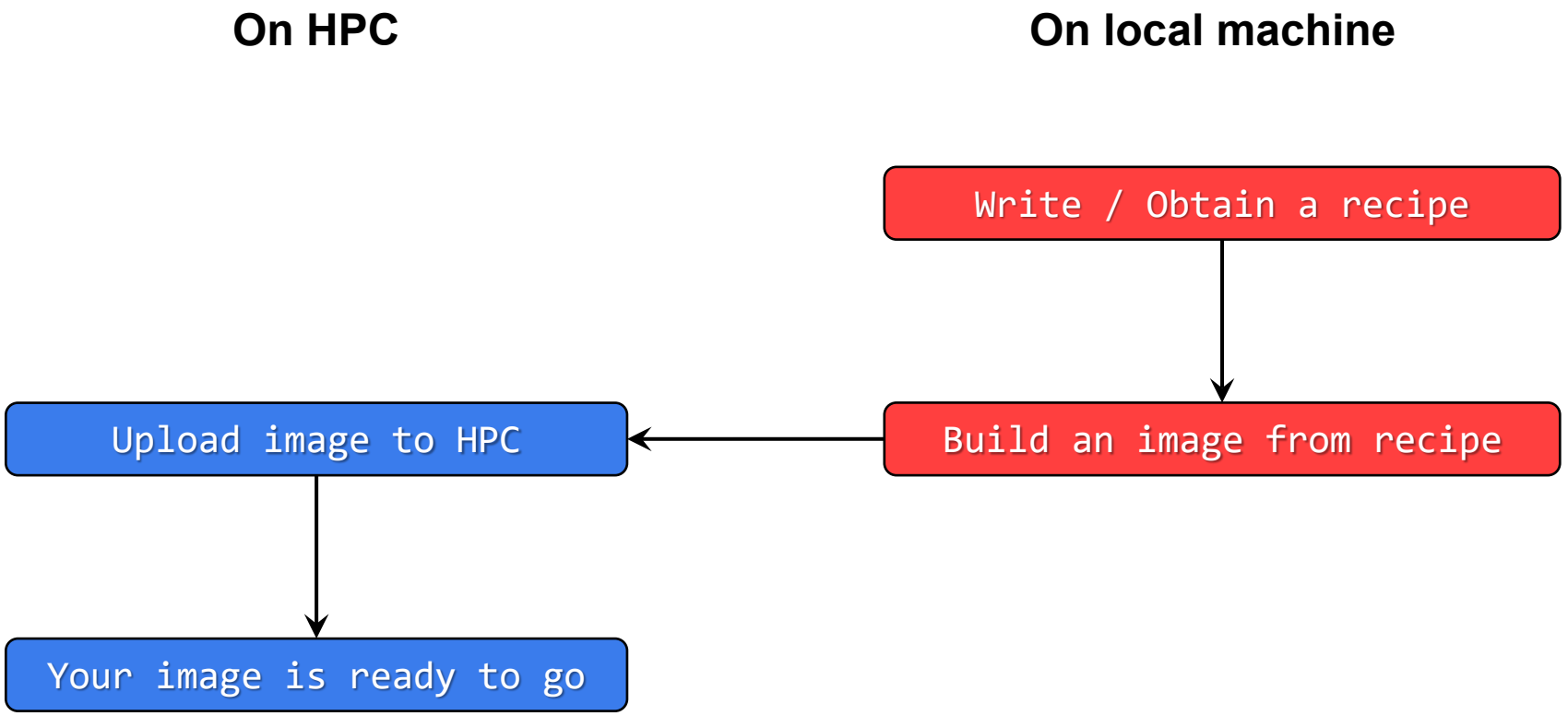
3) Make it easier - Recipe

- **Why?**



3) Make it easier - Recipe

- **Why?**



3) Make it easier - Recipe

a) What does a recipe look like?

ruby.def

```
BootStrap: docker
From: ubuntu:latest

%labels
Author       Jason Li
Description  A container with Ruby installed

%post
apt update
apt install -y ruby

%environment
export MYENV="Some environmental variable"

%runscript
ruby -e "puts 'Hello from container!'"
```

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Header
- Base image info (how, where, what to pull)

3) Make it easier - Recipe

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```

Label

- Container information (write whatever you want)

3) Make it easier - Recipe

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```

Post
- Commands to execute after the base image is pulled

3) Make it easier - Recipe

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```

Environment

- Define environmental variables every time the container is executed

3) Make it easier - Recipe

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Runscript
- Commands to be run with `singularity run`

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3) Make it easier - Recipe

b) Build the recipe

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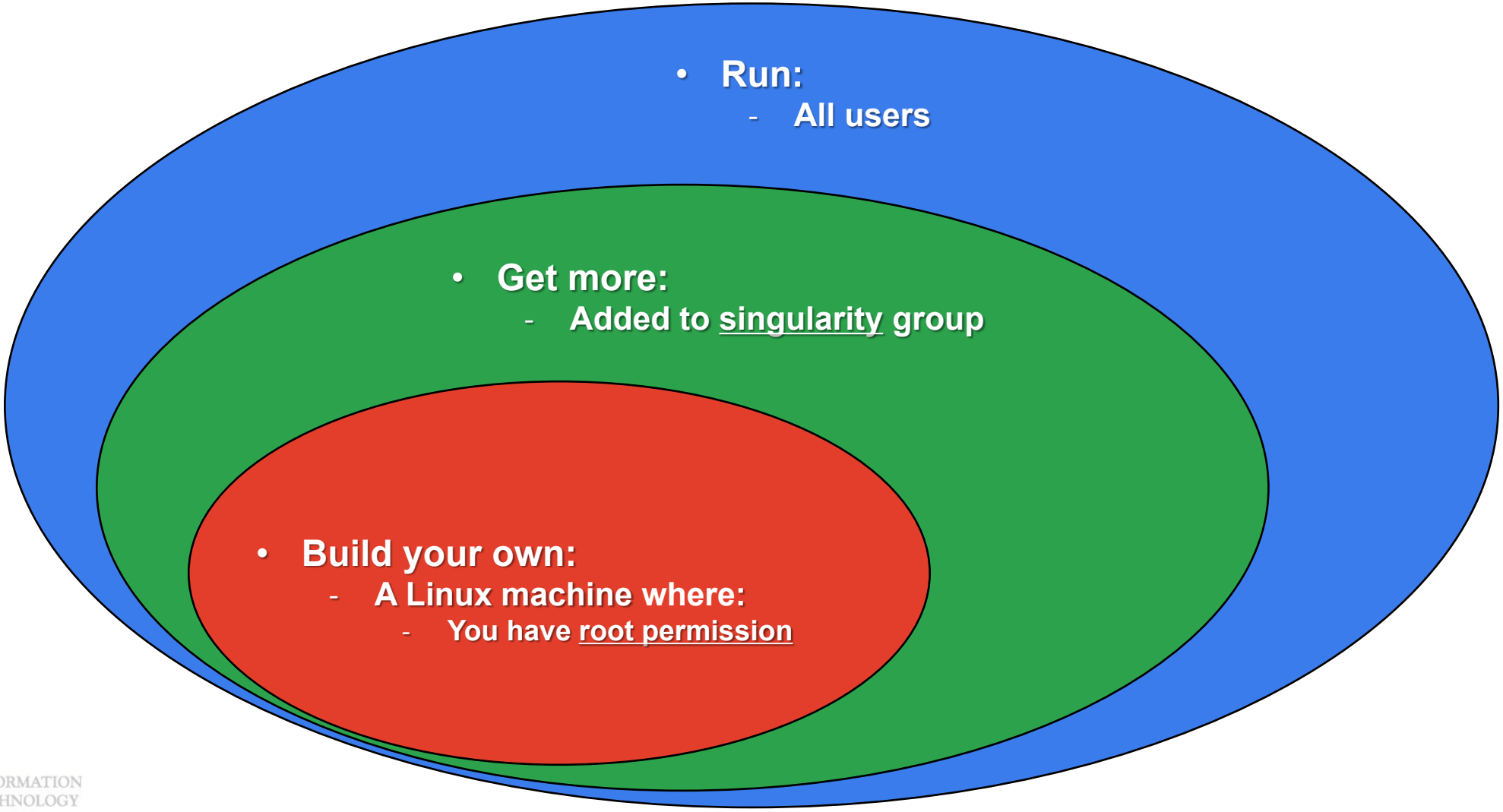
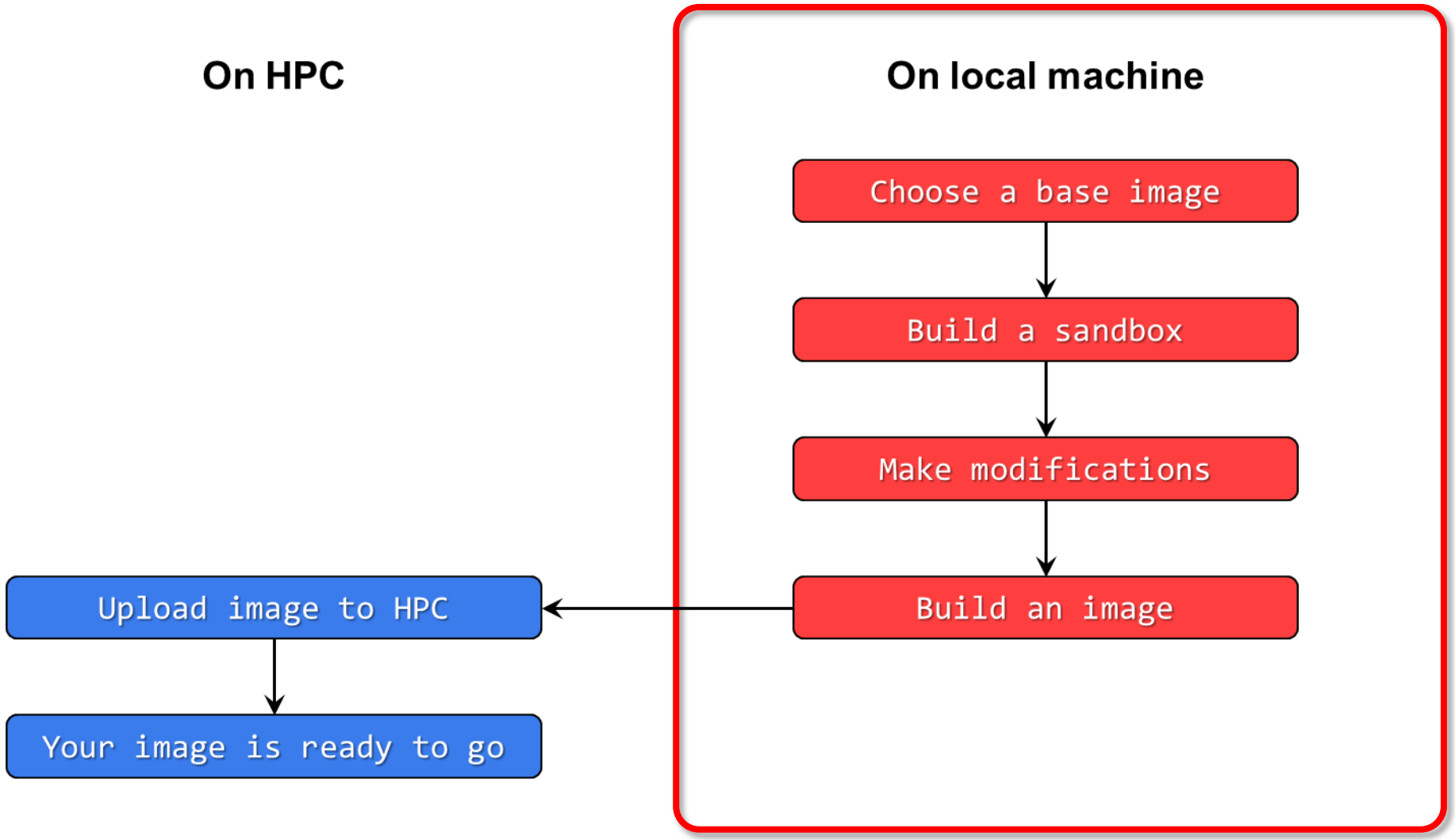
Summary


• Run:
- All users
• Get more:
- Added to singularity group
• Build your own:
- A Linux machine where:
- You have root permission

Summary


On HPC
On local machine
Choose a base image
Build a sandbox
Make modifications
Build an image
Upload image to HPC
Your image is ready to go

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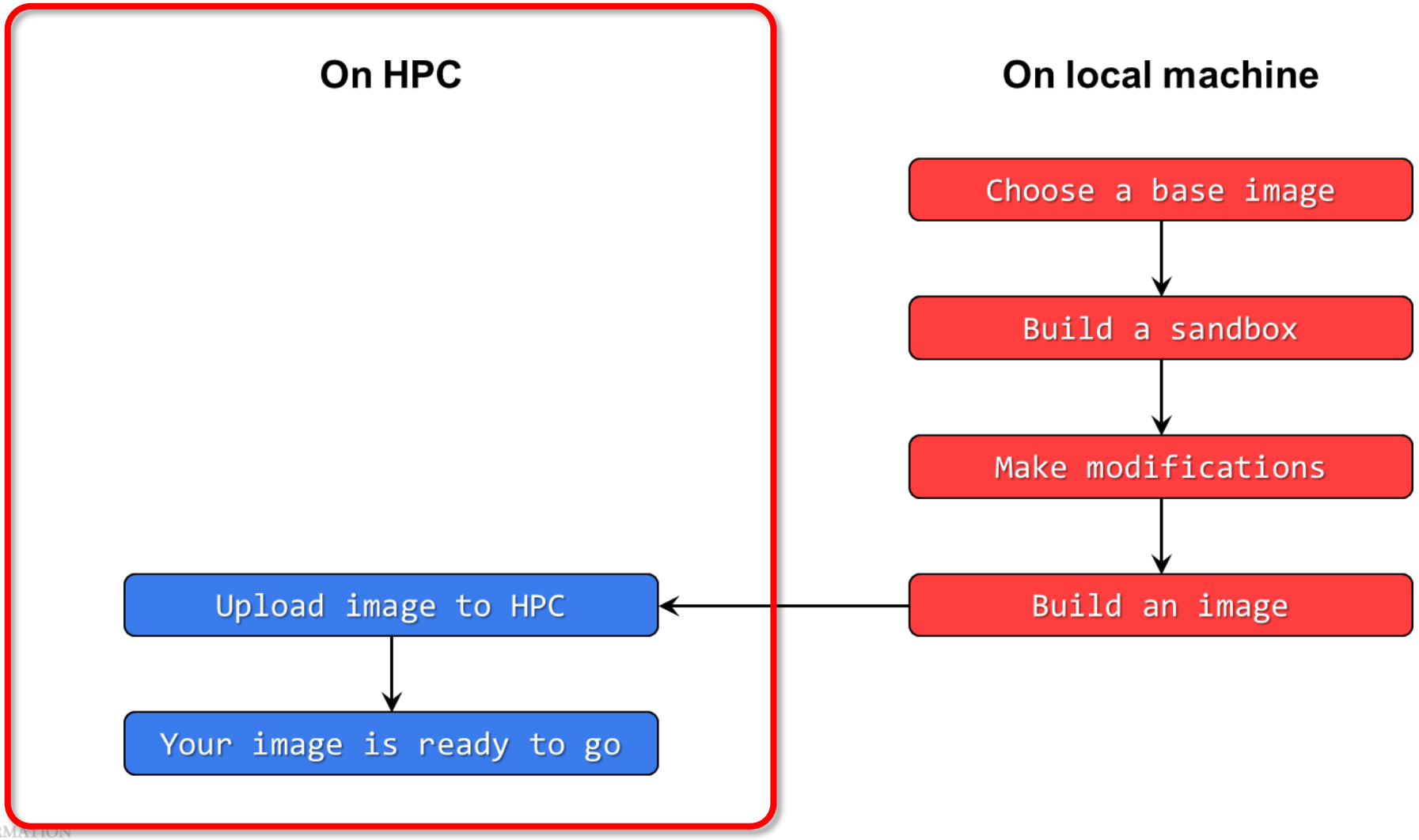
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Conclusion

Conclusion

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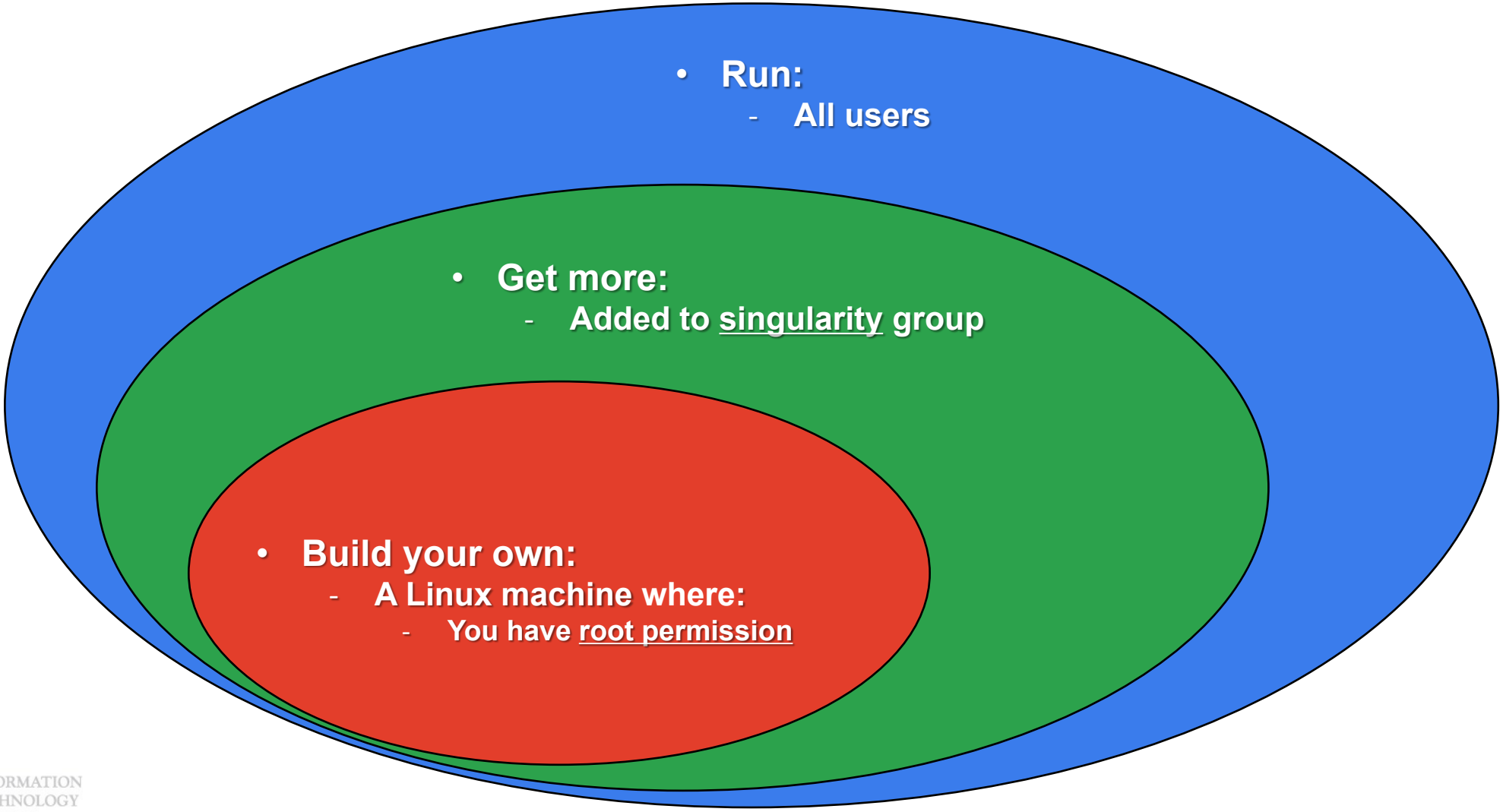
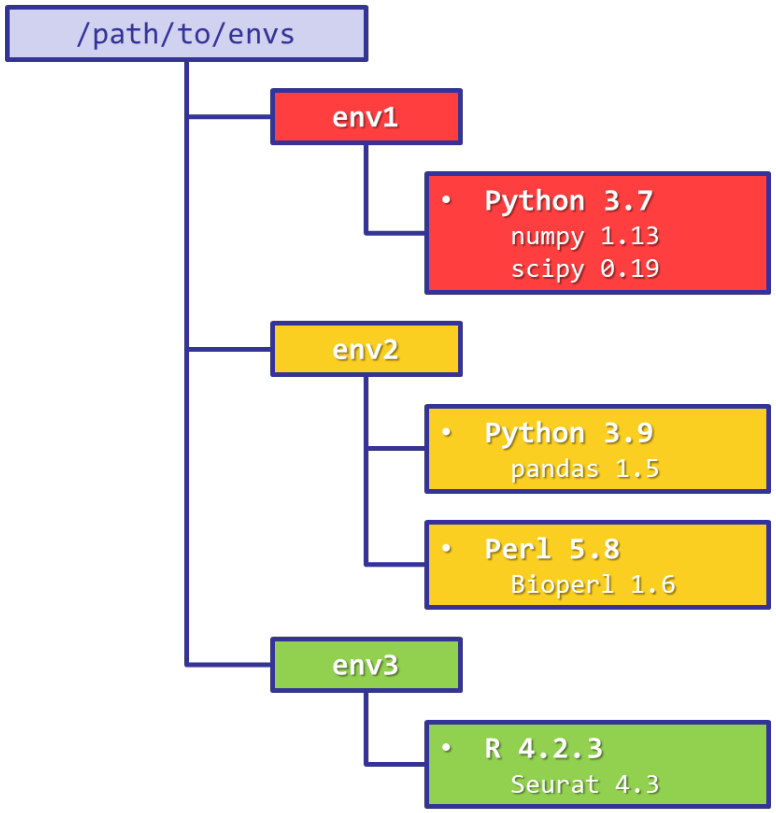
Take home message

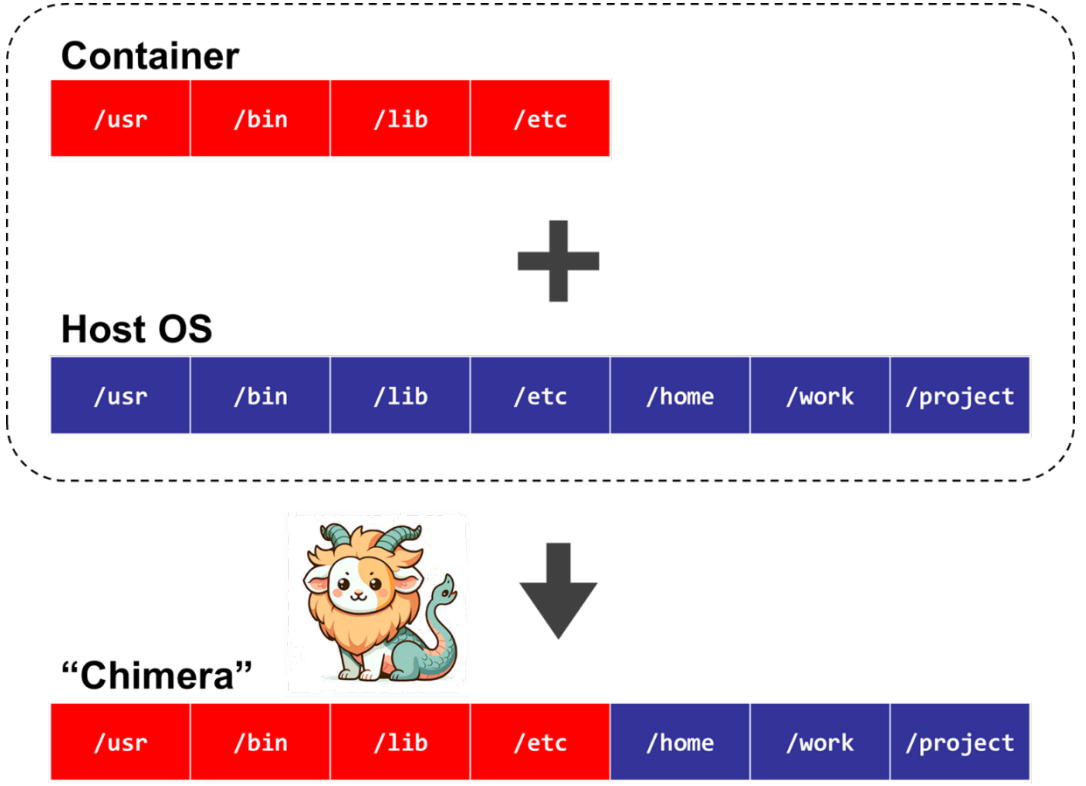


To conclude our mini series…

Conda vs Singularity

- **Virtual Environment** v.s. **Container** ?





Conda vs Singularity

	Conda / Virtual Environments	Singularity / Containers
Availability	All users	All users, but may need additional things
Self-contained	Yes	Yes
Isolated	Yes (but still accessible from outside)	Perfect (completely isolated from outside)
Editability	Yes	No (Must create a new image)
Disk usage	Large	Smaller
Portability	Possible (with .yml recipe)	Great (just copy-paste one file)
Security	Fair	Good
Ease of use	Good	May require a little more understanding

Conda vs Singularity

	Conda / Virtual Environments	Singularity / Containers
Good for	• Less hassle to create and install software from scratch • If you need to frequently make modifications	• Less hassle if the developer releases a working container • If you don't need to make changes after it is created • Portability • Reduce disk usage • Your system admins yelled at you about security risk

Contact us

- **Contact user services**
  - Email Help Ticket: sys-help@loni.org
  - Telephone Help Desk: +1 (225) 578-0900

“Commercial” time!

- **Are you tired of wring the long, tedious singularity commands?**

```
$ singularity exec --nv -B /work,/project,/usr/local/package \
    /home/admin/singularity/ubuntu-training.sif \
    python helloworld.py
```

“Commercial” time!

- Try **SIMPLE-MOD** !
  - https://github.com/lsuhpchelp/SIMPLE-MOD
  - A GUI tool to create module key from container-based software.
  - Using the software in containers is as easy as:

```
$ module load busco
$ busco --version
  BUSCO 5.6.1
```