Magic Tools to Install & Manage Software

ingularity Container

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Outlines

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

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1. **Why Container?**
   1) Problems
   2) Container & Singularity
2. **Run an Existing Container Image**
   1) Basic commands
   2) Running jobs with Singularity
3. **Get More Container Images**
   1) Where to get
   2) Basic commands
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:**

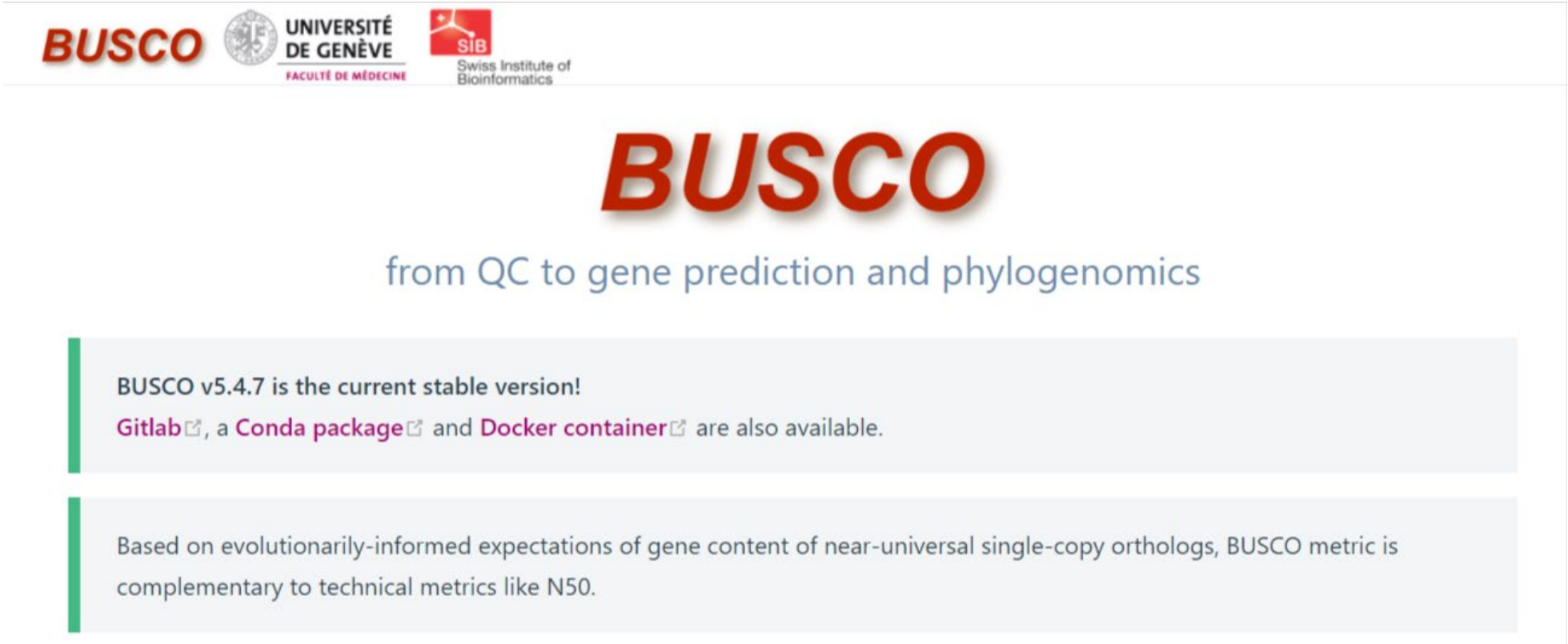
Installing software on an HPC system

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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- https://github.com/smirarab/sepp/
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- Dependencies

The following dependencies are required for AUGUSTUS:

- for gzip compressed input: (set ZIPINPUT = false in common.mk if t… are 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!)

```
[jasonli3@mike4 ~]$ module load python
[jasonli3@mike4 ~]$ pip install gdal
```

1) Problems

b) Permission denied (Welcome to HPC!)

```
Using numpy 2.0.2
running egg_info
writing gdal-utils/GDAL.egg-info/PKG-INFO
writing dependency_links to gdal-utils/GDAL.egg-info/dependency_links.txt
writing entry points to gdal-utils/GDAL.egg-info/entry_points.txt
writing requirements to gdal-utils/GDAL.egg-info/requires.txt
writing top-level names to gdal-utils/GDAL.egg-info/top_level.txt
Traceback (most recent call last):
  File "<string>", line 91, in fetch_config
  File "/usr/local/packages/python/3.9.7-anaconda/lib/python3.9/subprocess.p
    self._execute_child(args, executable, preexec_fn, close_fds,
  File "/usr/local/packages/python/3.9.7-anaconda/lib/python3.9/subprocess.p
    raise child_exception_type(errno_num, err_msg, err_filename)
FileNotFoundError: [Errno 2] No such file or directory: 'gdal-config'
```

1) Problems

b) Permission denied (Welcome to HPC!)

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    raise child_exception_type(errno_num, err_msg, err_filename)
FileNotFoundError: [Errno 2] No such file or directory: 'gdal-c
```

libgdal

1) Problems

b) Permission denied (Welcome to HPC!)

- If you ask Google / AI…

```
$ sudo yum install libgdal-devel        # On Red Hat

$ sudo apt-get install libgdal-dev      # On Ubuntu
```

1) Problems

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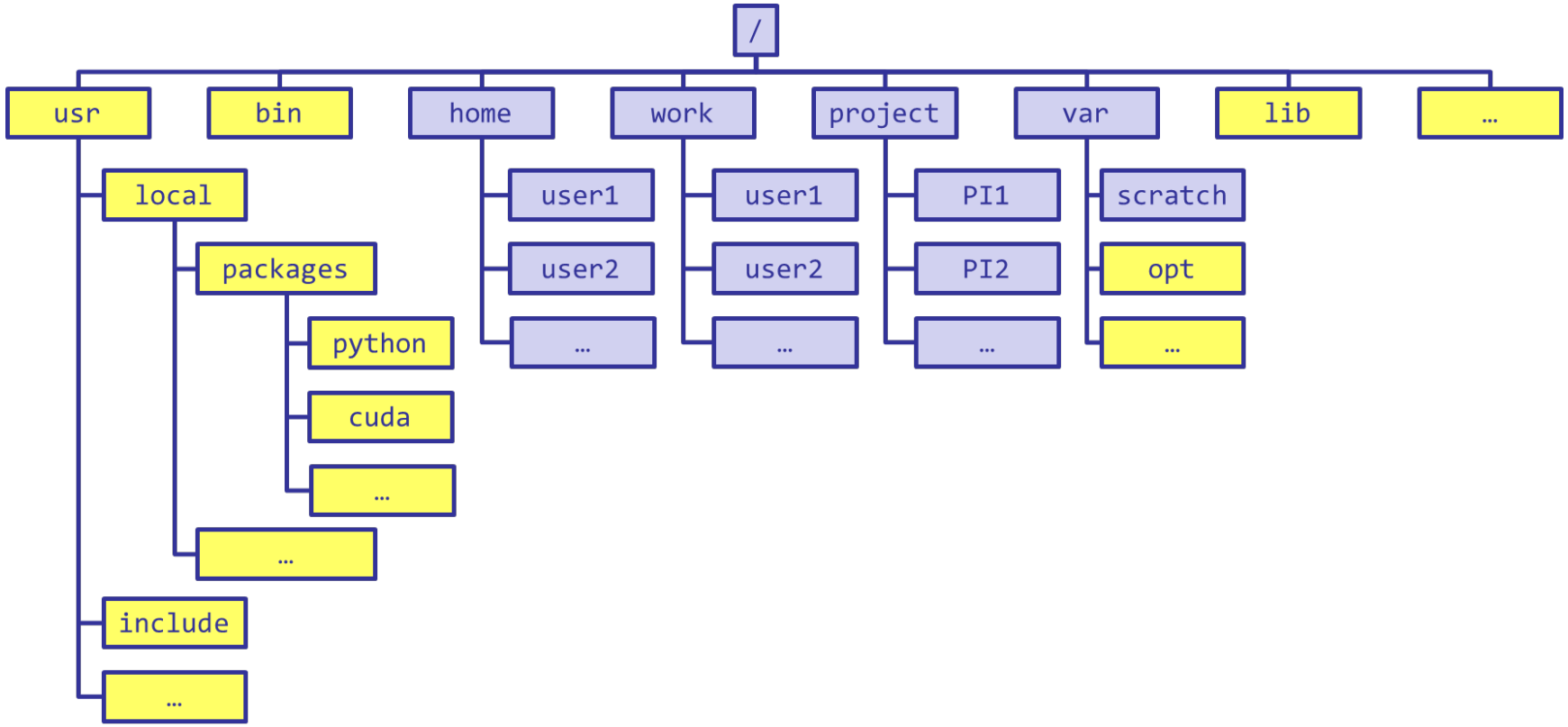


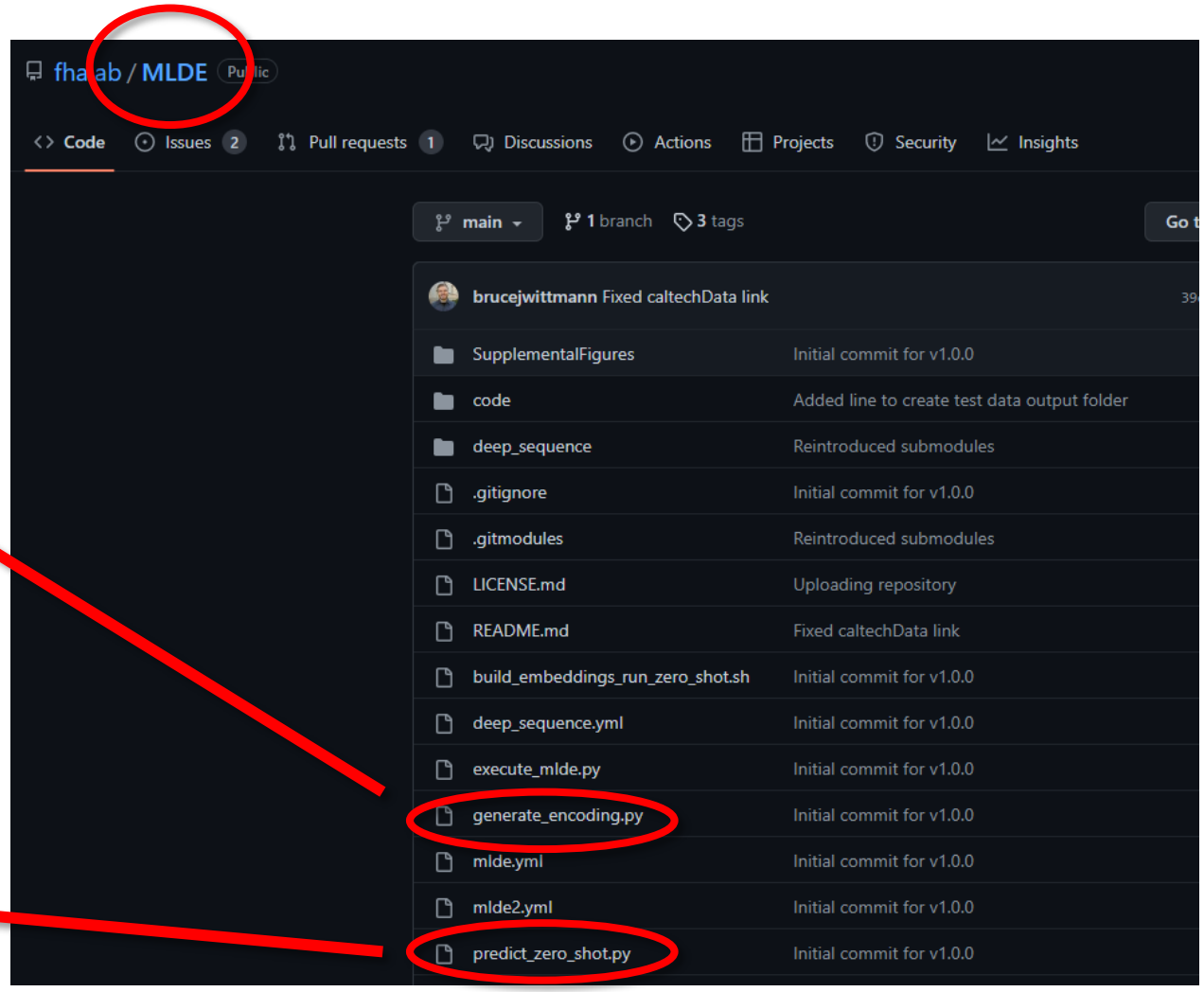
1) Problems

c) Conflicted packages

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

Tensorflow 1.13

PyTorch > 1.5



d) Sharing / Migrating your software

– 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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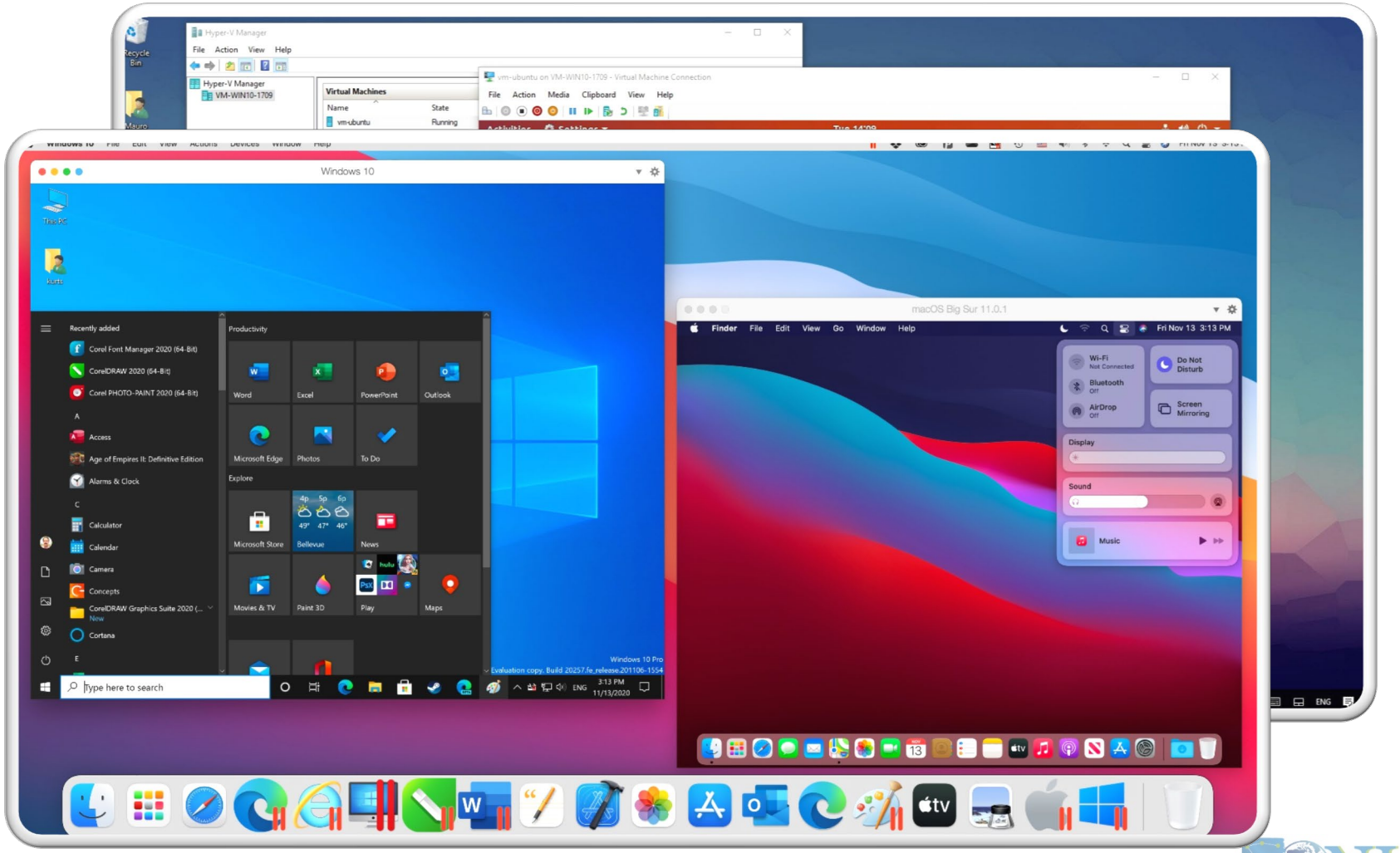
2) Container & Singularity

a) What is a container?

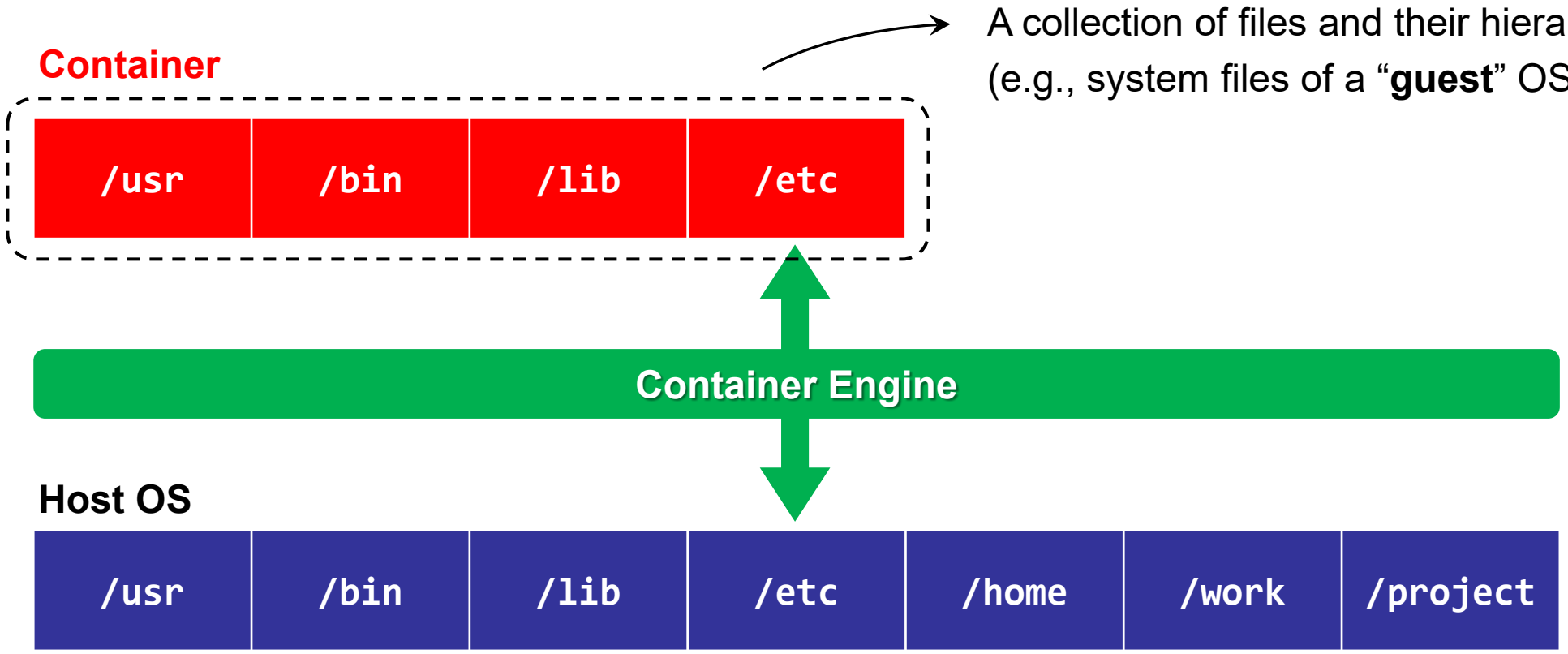
- **Virtual machine**
  - "Virtualize" / "mimic" an **entire computer** on another computer
  - Virtualize both **hardware** and **software**



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**

a) What is a container?

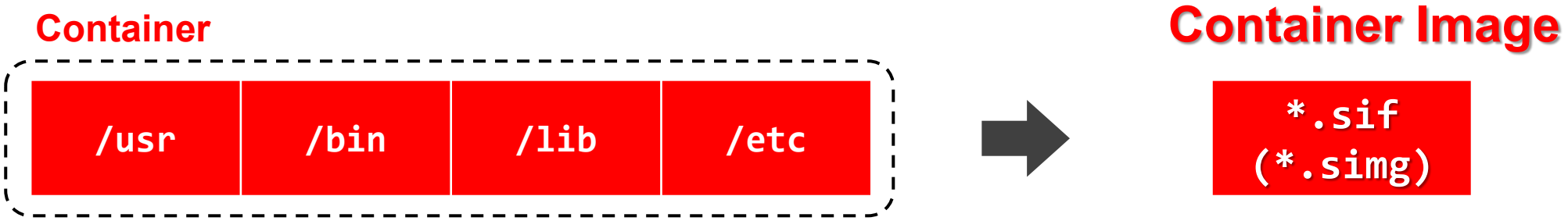


a) What is a container?

/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

a) What is a container?

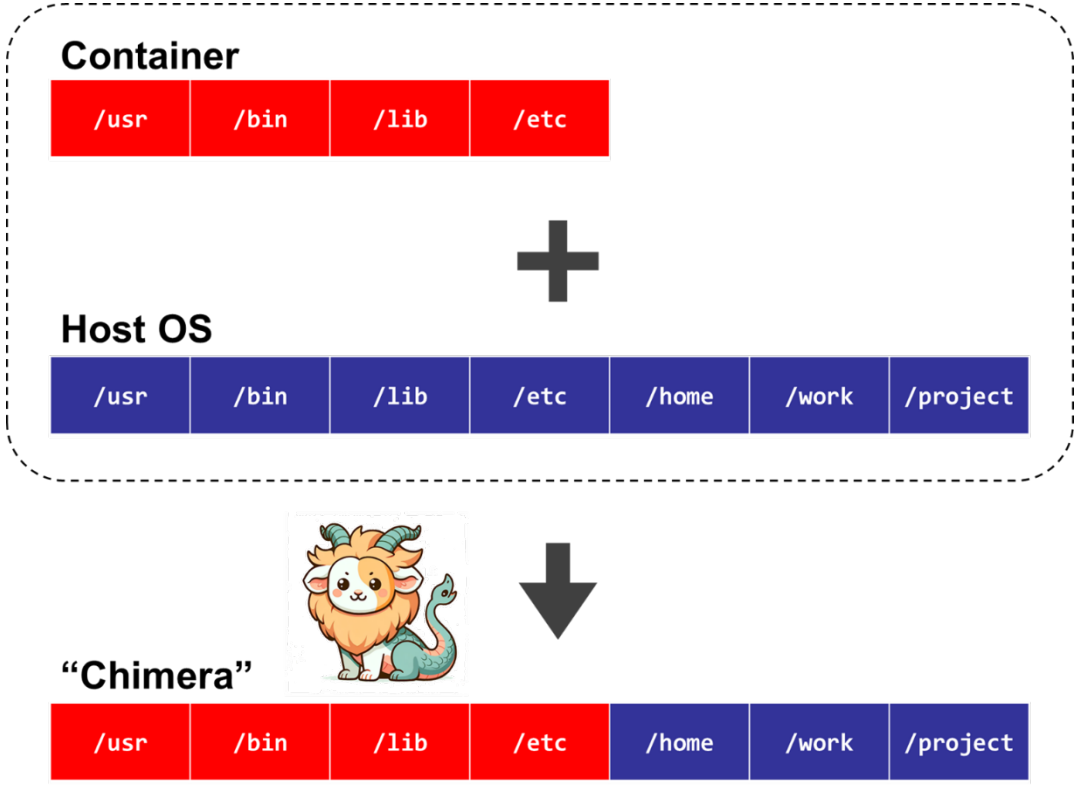


a) What is a container?

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

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

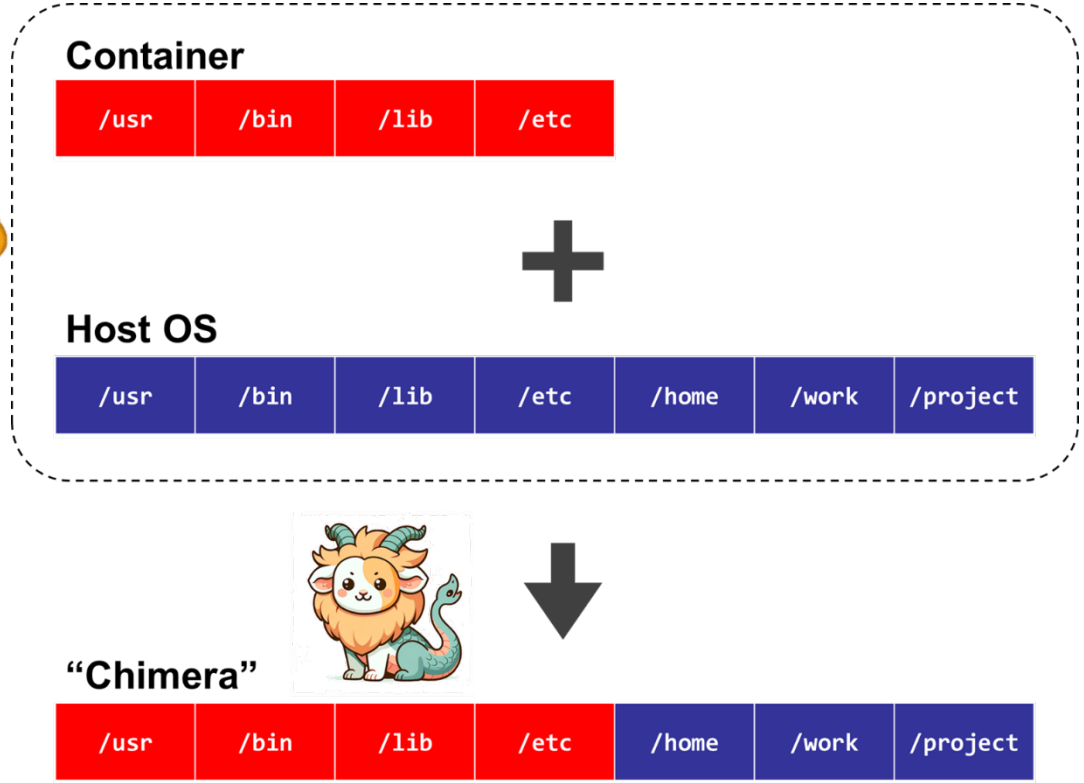
    Whatever happens in a container stays in that container…



b) How does it solve my problems?

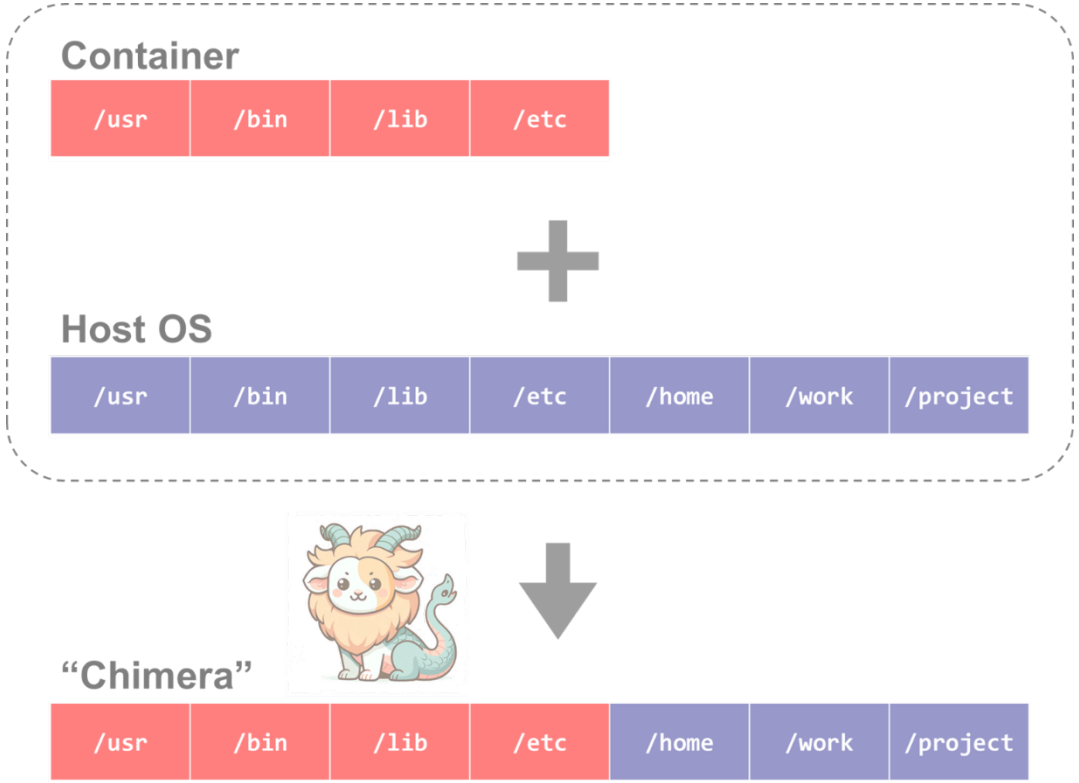
- **Dependency issue**
  - Pack all dependencies (even OS) in container
  - Can use `apt-get` or `yum`
  - **Developers now release containers!**

- **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?

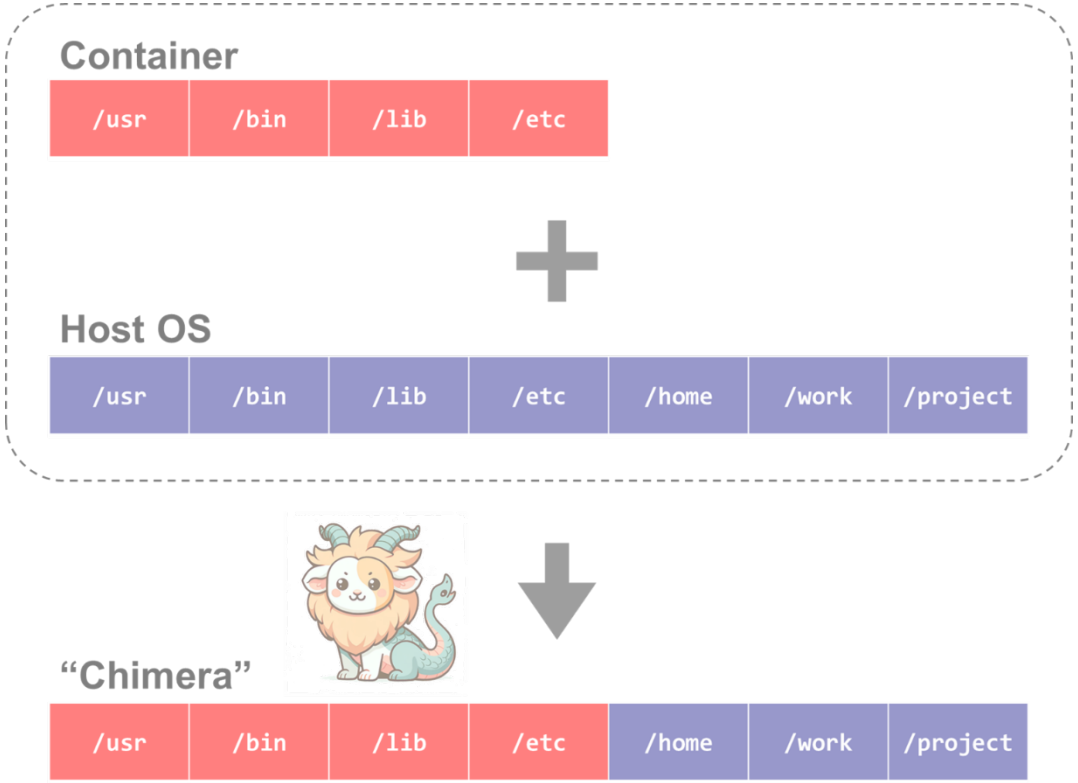
Technology →



c) What is Singularity?

Singularity

↑ **Software** system that implements the technology



c) What is Singularity?

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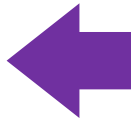


- Does **NOT** need root privileges
- "**Container for HPC**"

- **Needs** root privileges

d) Singularity availability

i. On all clusters

- ✓ **LSU HPC**: SMIC, Deep Bayou, Supermike 3
- ✓ **LONI**: QB-3, QB-4

ii. Only on computing nodes

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

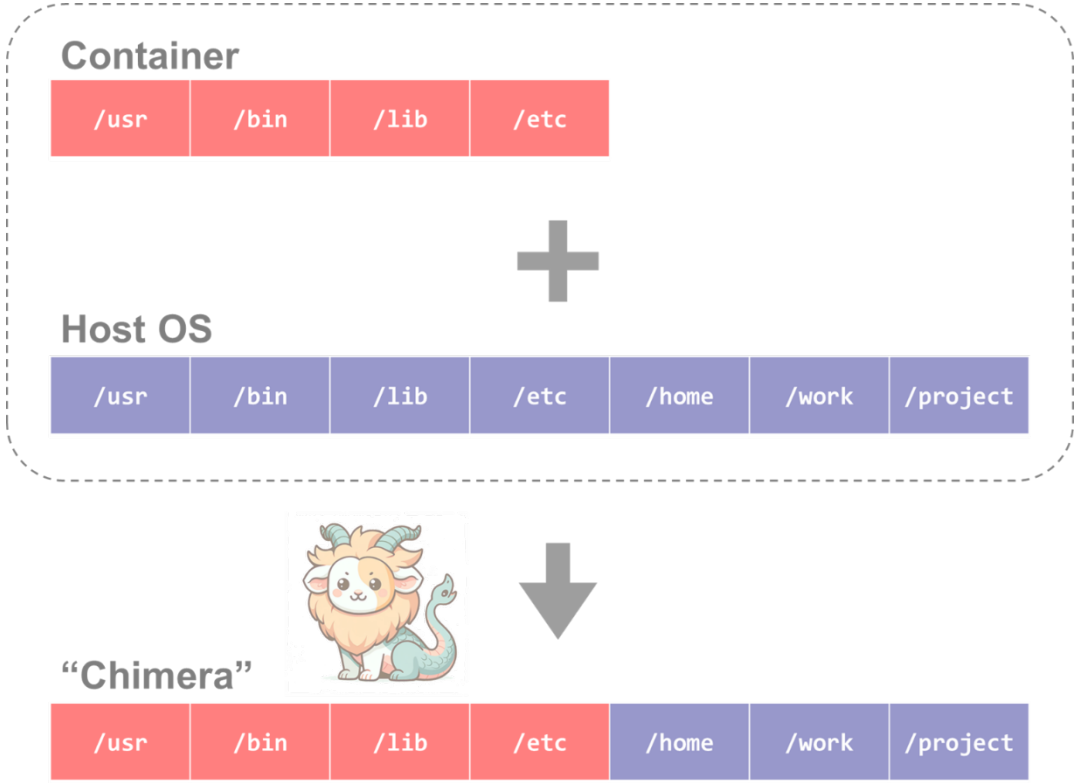
iii. To all users

- × No additional action required

Summary

Technology that helps with software installation →

↓ **Software** system that implements the technology



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1) Basic commands

- **Available images**

  – On all clusters: `/project/containers/images`

```
(base) [jasonli3@qbd4 ~]$ ls /project/containers/images/
agat-1.4.0.sif                          fed28.simg
alphafold-catgumag-2.2.sif              fenics-adjoint.2018.ubuntu16.simg
alps-2.3.0-dockerhub.simg               firedrake.dockerhub.simg
alps-2.3.0-dockerhub-v2.simg            firedrake.vanilla.simg
bcftools-1.18.sif                       fmriprep-1.1.8-ubuntu-16.0.4.simg
beast2-2.7.7.sif                        fmriprep-1.3.2-ubuntu-16.0.4.simg
blast-2.14.1.sif                        gatk-4.5.0.0.sif
blender-2.79b-cuda-8.0-ubuntu-16.04.simg gcc-9.2.0-dockerhub.simg
bowtie2-2.5.1.sif                       hisat2-2.2.1.sif
braker-3.0.8.sif                        jax-0.4.26.sif
busco-5.7.1.sif                         jax.sif
bwa-0.7.17.sif                          maker-3.01.03.sif
```

1) Basic commands

a) Open an interactive shell in the image

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

Try me: `/project/containers/images/ubuntu-training.sif`

1) Basic commands

a) Open an interactive shell in the image

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

b) Execute a single command in the image

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

Try me: `/project/containers/images/ubuntu-training.sif`

1) Basic commands

b) 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

1) Basic commands

c) Run a prewritten script (less common)

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

1) Basic commands

- **Quick recap**

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

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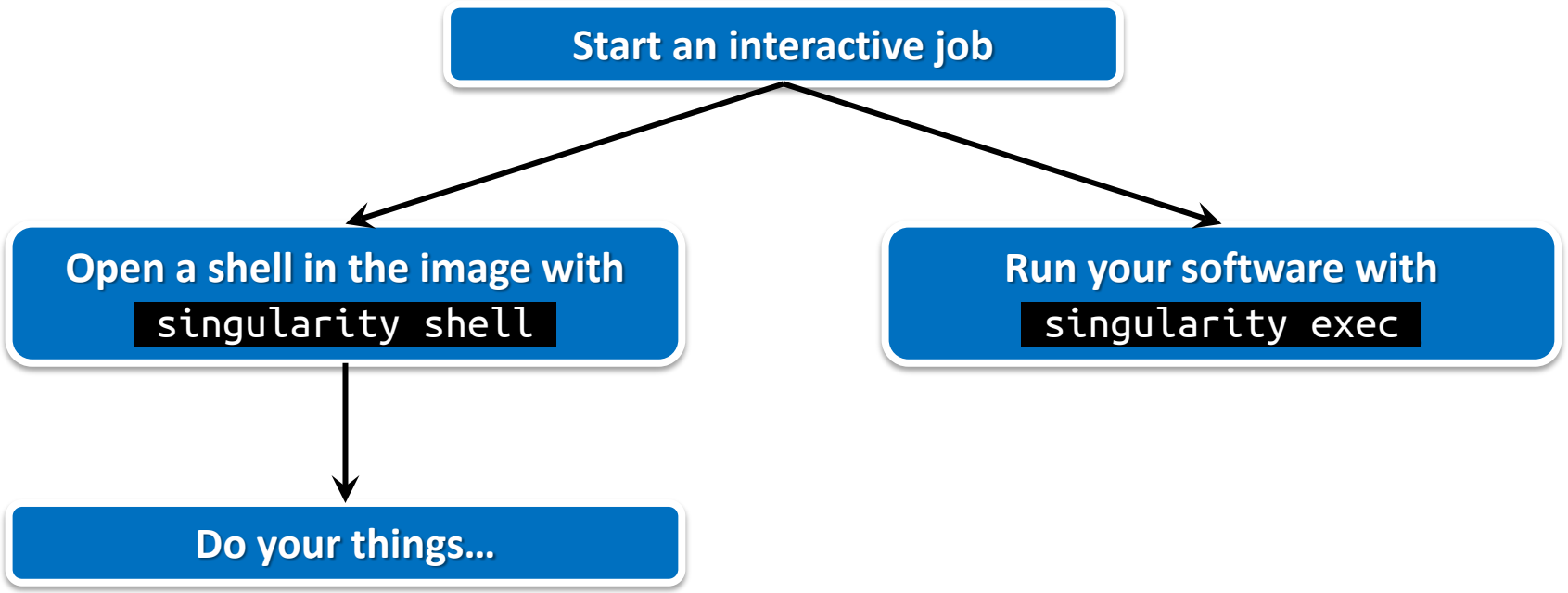
2) Run jobs with Singularity

- **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

2) Run jobs with Singularity

a) Interactive job



2) Run jobs with Singularity

b) Batch job

```
#!/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

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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Get More Container Images

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alphafold-catgumag-2.2.sif              fenics-adjoint.2018.ubuntu16.simg
alps-2.3.0-dockerhub.simg               firedrake.dockerhub.simg
alps-2.3.0-dockerhub-v2.simg            firedrake.vanilla.simg
bcftools-1.18.sif                       fmriprep-1.1.8-ubuntu-16.0.4.simg
beast2-2.7.7.sif                        fmriprep-1.3.2-ubuntu-16.0.4.simg
blast-2.14.1.sif                        gatk-4.5.0.0.sif
blender-2.79b-cuda-8.0-ubuntu-16.04.simg gcc-9.2.0-dockerhub.simg
bowtie2-2.5.1.sif                       hisat2-2.2.1.sif
braker-3.0.8.sif                        jax-0.4.26.sif
busco-5.7.1.sif                         jax.sif
bwa-0.7.17.sif                          maker-3.01.03.sif
```

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1) 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 !**


techradar pro THE BUSINESS TECHNOLOGY EXPERTS US Edition

News Reviews Features Expert Insights Website builders Web hosting

TRENDING Expert Insights Best web hosting Best website builder

When you purchase through links on our site, we may earn an affiliate commission. Here's how it works.

Pro > Security

Malware attacks on Docker Hub spread millions of malicious repositories

News By Sead Fadilpašić published yesterday

Millions of repositories contained nothing but links to malicious websites

[1] https://www.techradar.com/pro/security/malware-attacks-on-docker-hub-spread-millions-of-malicious-repositories

1) 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 trustworthy icons like Docker Official Image or Verified Publisher • Avoid third-party publishers that you don't know

Outlines

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

2) Basic Commands

a) Simple version

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

2) Basic Commands

b) Advanced version

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)

2) Basic Commands

- **Quick recap**

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

2) Basic Commands

- **BONUS: Hot packages!**

  i. **PyTorch** (**2.8.0**, w/ GPU support)

```
$ singularity pull docker://pytorch/pytorch:2.8.0-cuda12.9-cudnn9-runtime
```

  ii. **Tensorflow** (**2.17.0 ***, w/ GPU support)

```
$ singularity pull docker://tensorflow/tensorflow:2.17.0-gpu-jupyter
```

* *2.17.0 is the latest **working** official container, but not the latest version (2.20.0). Tensorflow develop team has not updated CUDA support in their official container over a year for unknown reason…*

2) Basic Commands

- **BONUS: Hot packages!**

  i. **PyTorch** (**2.6.0**, w/ GPU support)

```
$ module load pytorch
```

  ii. **Tensorflow** (**2.16.1**, w/ GPU support)

```
$ module load tensorflow
```

Summary

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

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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).

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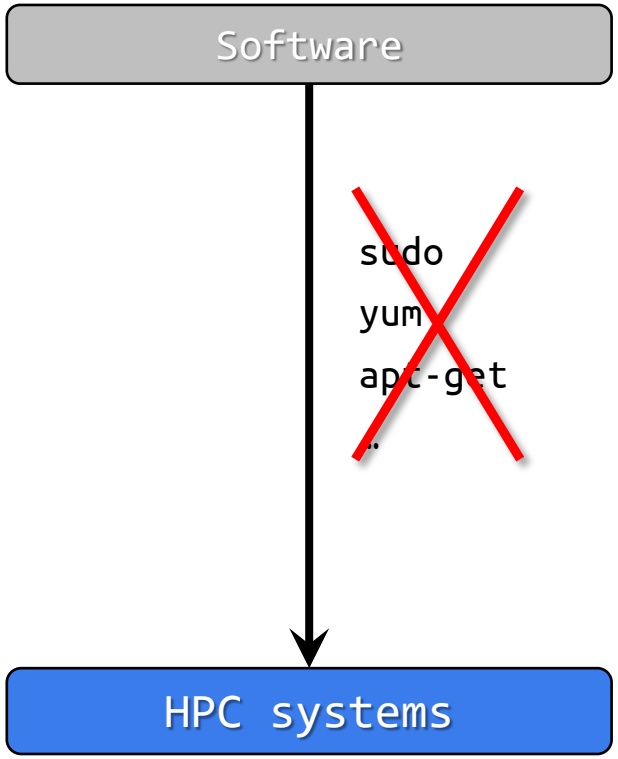
1) What you need

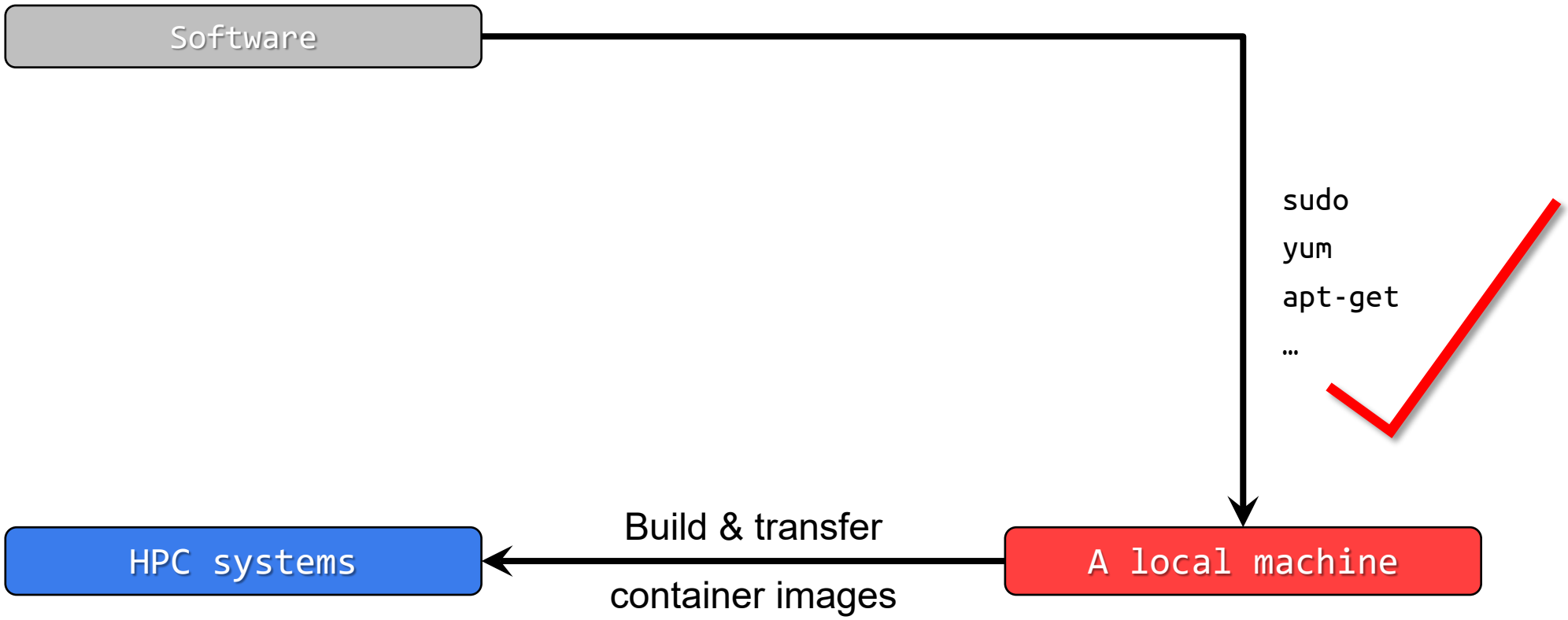
a) What you need:

A Linux machine w/ root privilege

b) Idea

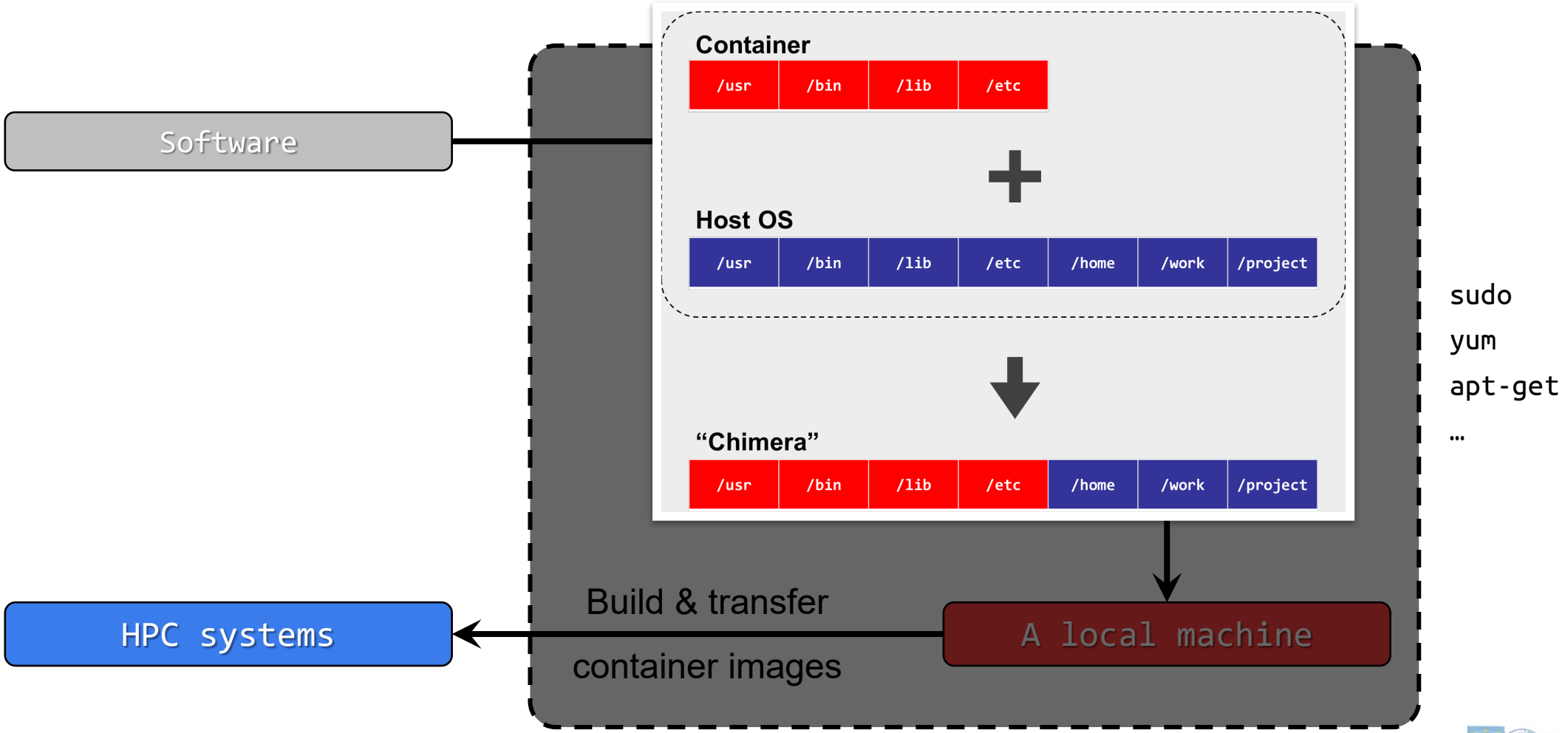


b) Idea

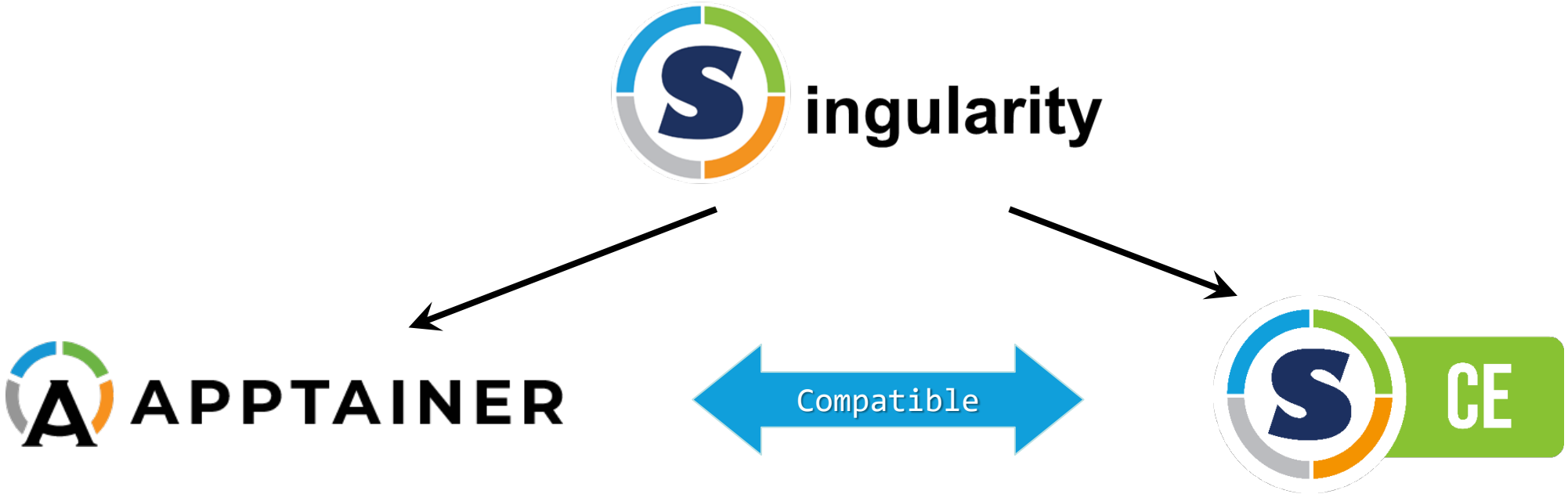

Software
sudo
yum
apt-get
…
HPC systems
Build & transfer
container images
A local machine

1) What you need

b) Idea



c) 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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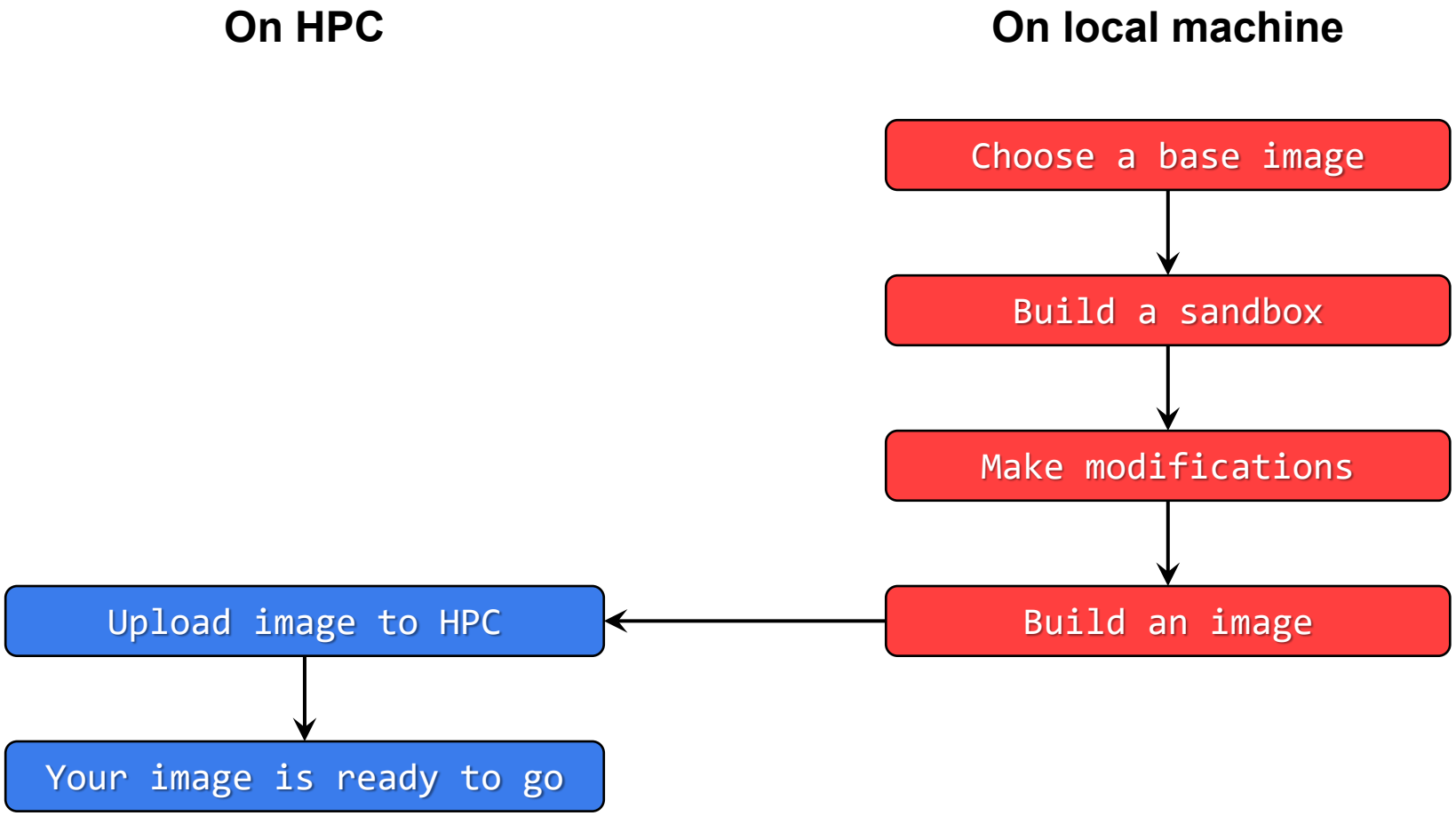
2) Typical workflow



2) Typical workflow

a) Choose a base image

Common choices	Typical scenarios
A minimum, "vanilla" 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)

2) Typical workflow

b) Build a sandbox

– What's a **sandbox** ?

- A **directory** form of a container (instead of a single, binary image file)
- 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

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

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

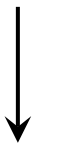
```
$ singularity build [options] <target> <source>
```

<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

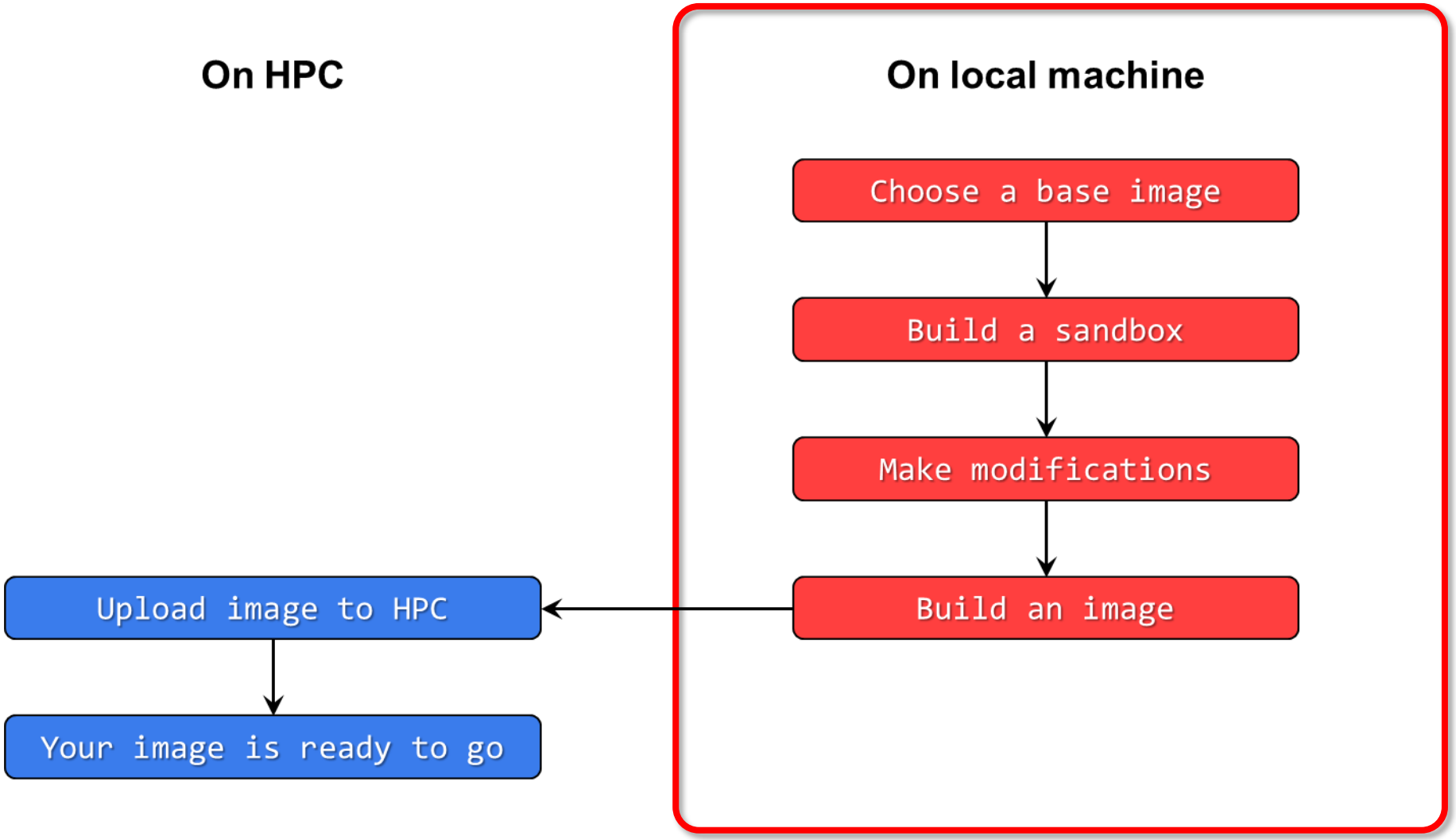
- **Quick recap**

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 ...`

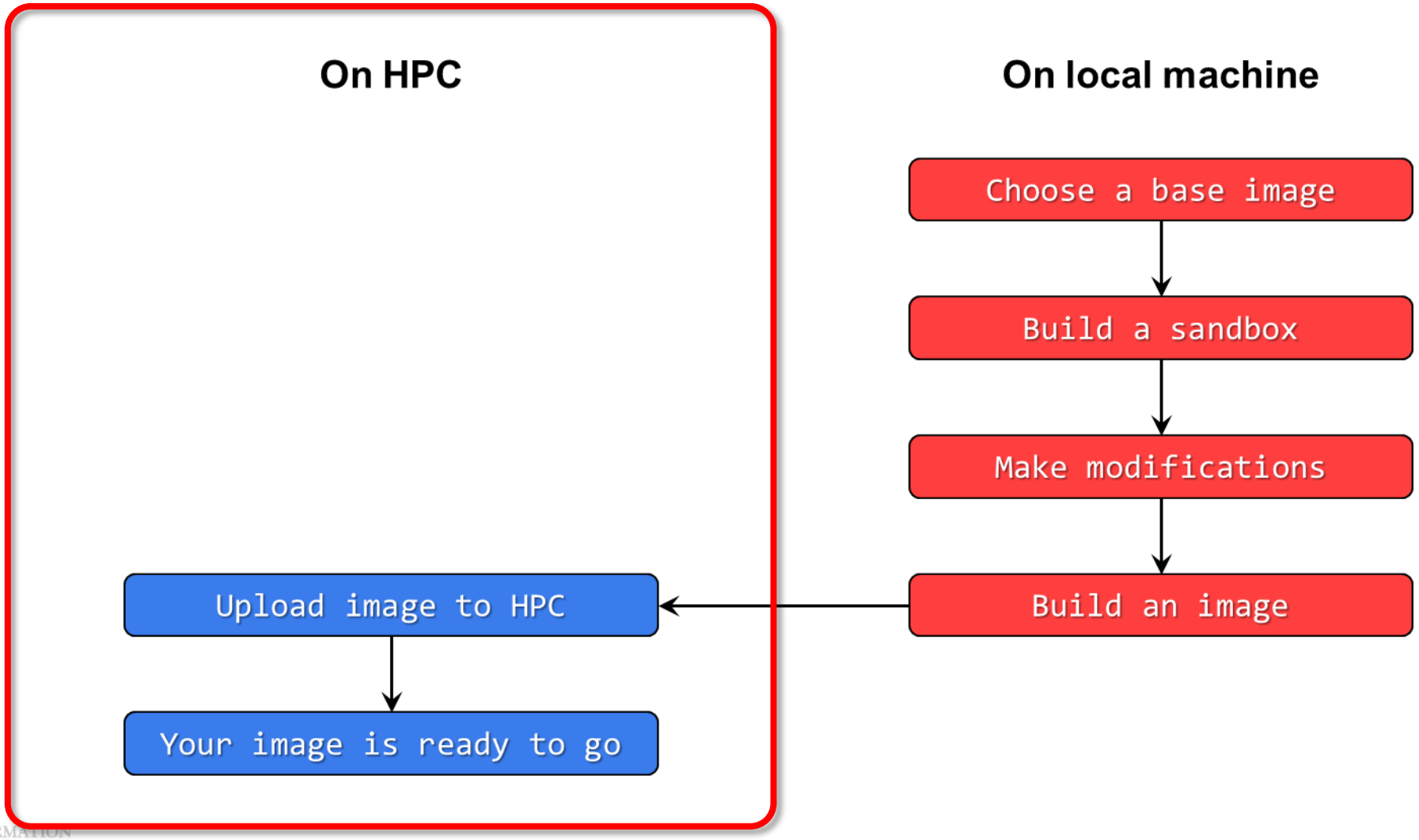
e) Upload image to HPC and run

Now! The moment of truth!

2) Typical workflow



2) Typical workflow



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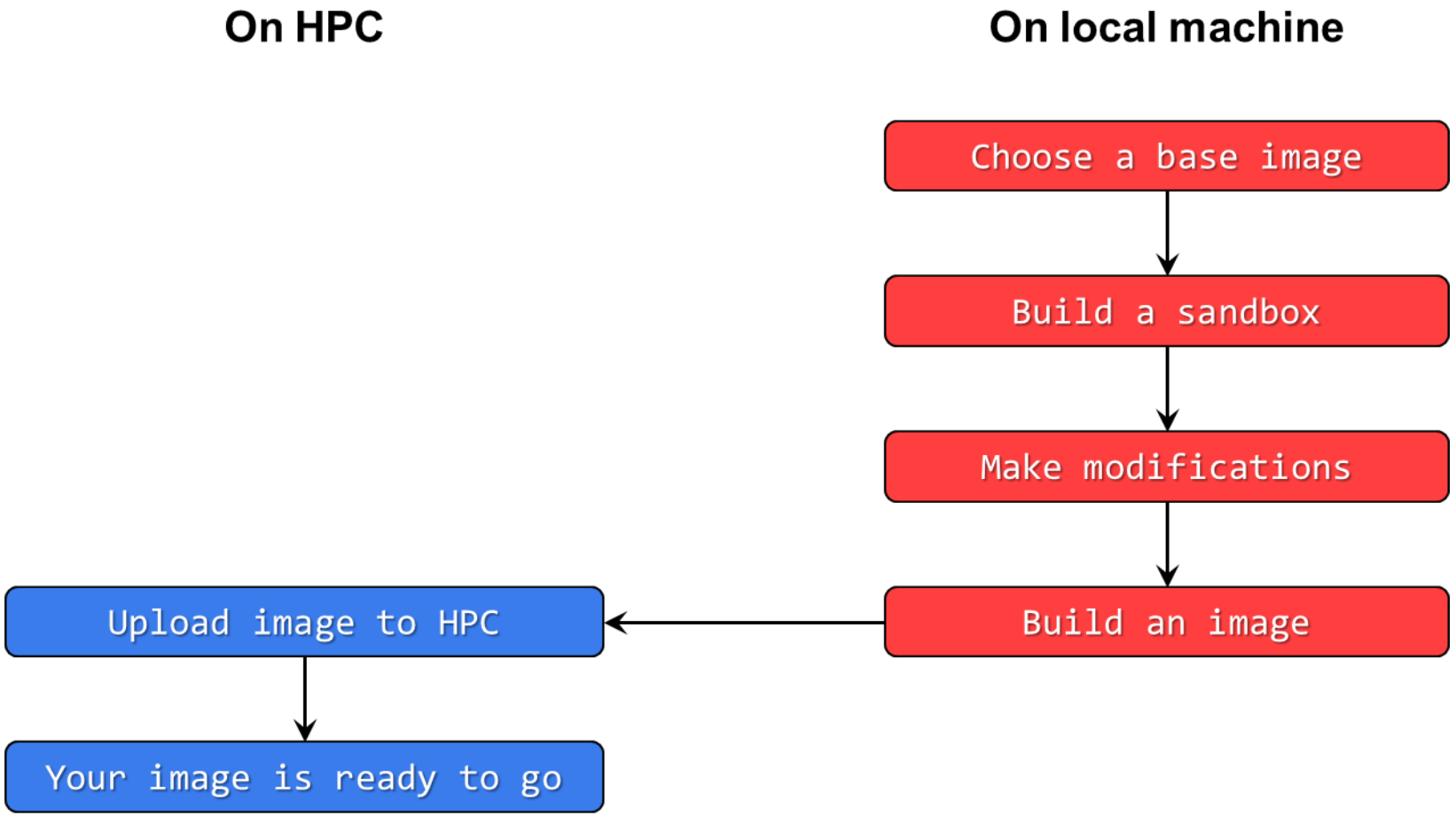
3) Make it easier - Recipe

- **Why?**



3) Make it easier - Recipe

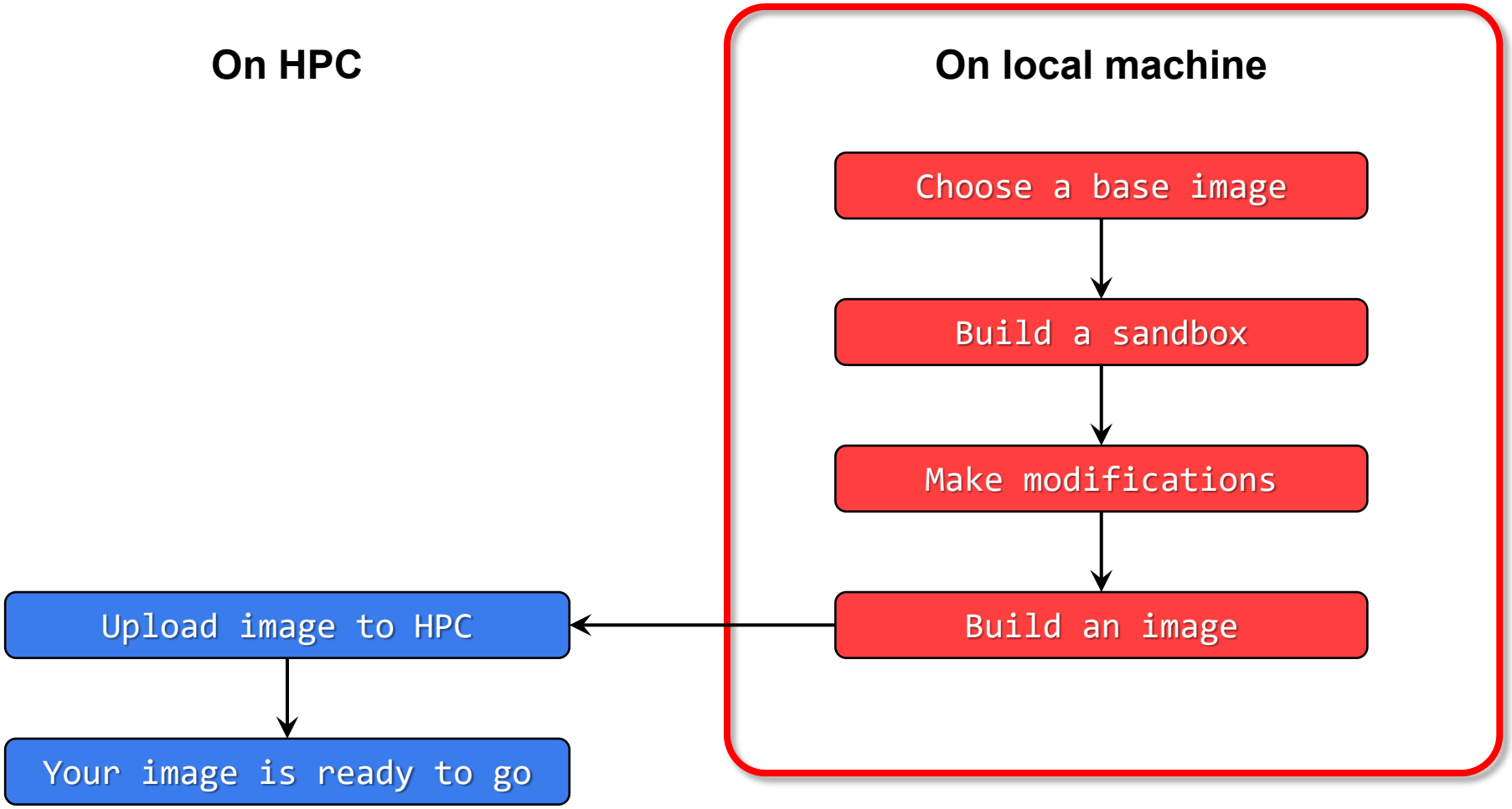
- **Why?**

Pros	Cons
• Flexibility	• Repeatability • Minimizing image size

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

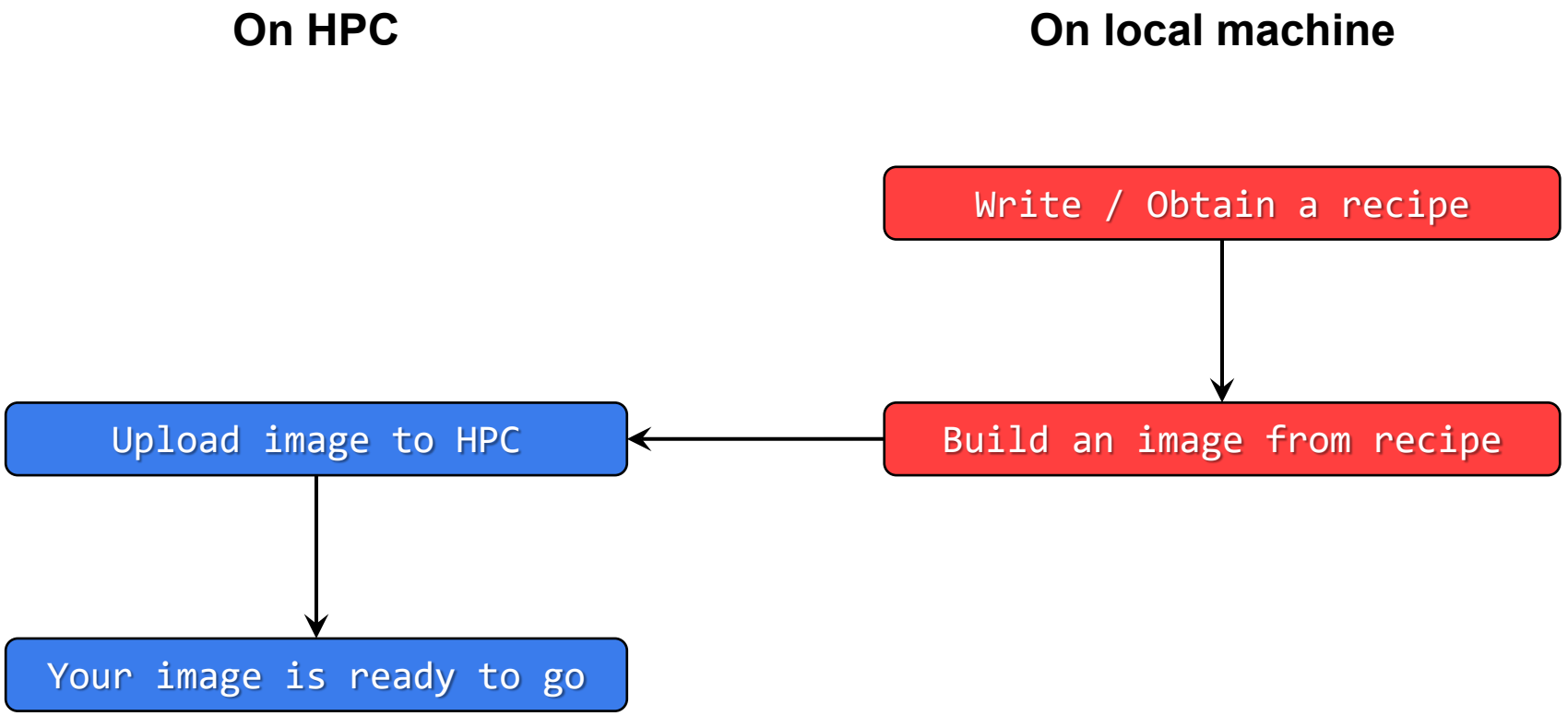
3) Make it easier - Recipe

- **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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BootStrap: docker
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apt update
apt install -y ruby

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

Environment

- Define environmental variables every time the container is executed

3) Make it easier - Recipe

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ruby.def

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From: ubuntu:latest

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%post
apt update
apt install -y ruby

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export MYENV="Some environmental variable"

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

Runscript
- Commands to be run with `singularity run`

3) Make it easier - Recipe

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ruby.def

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```

3) Make it easier - Recipe

b) Build the recipe

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

<source>	docker://container[:tag]	Build from a Docker container
	container_image.sif	Build from a local image file
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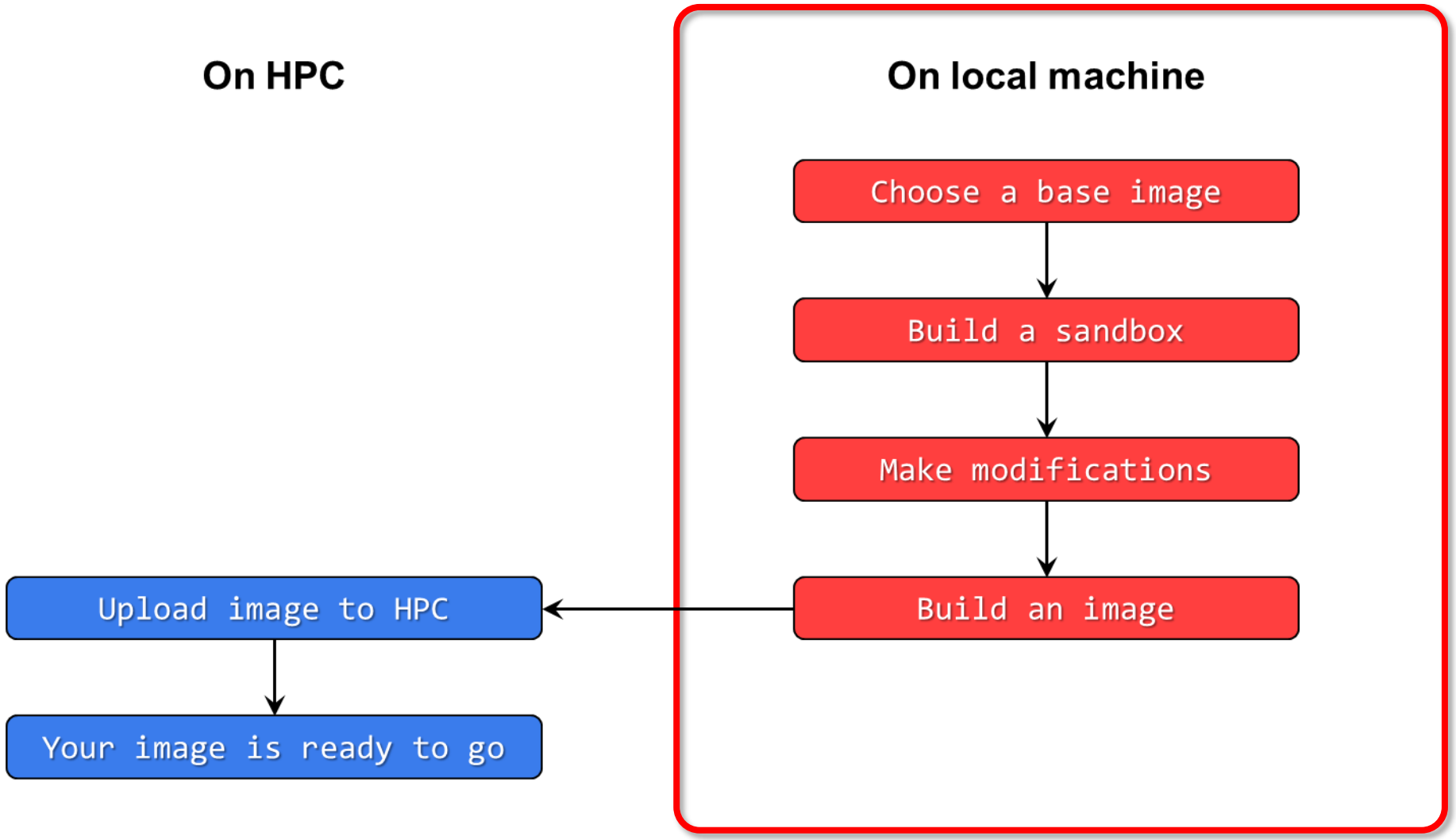
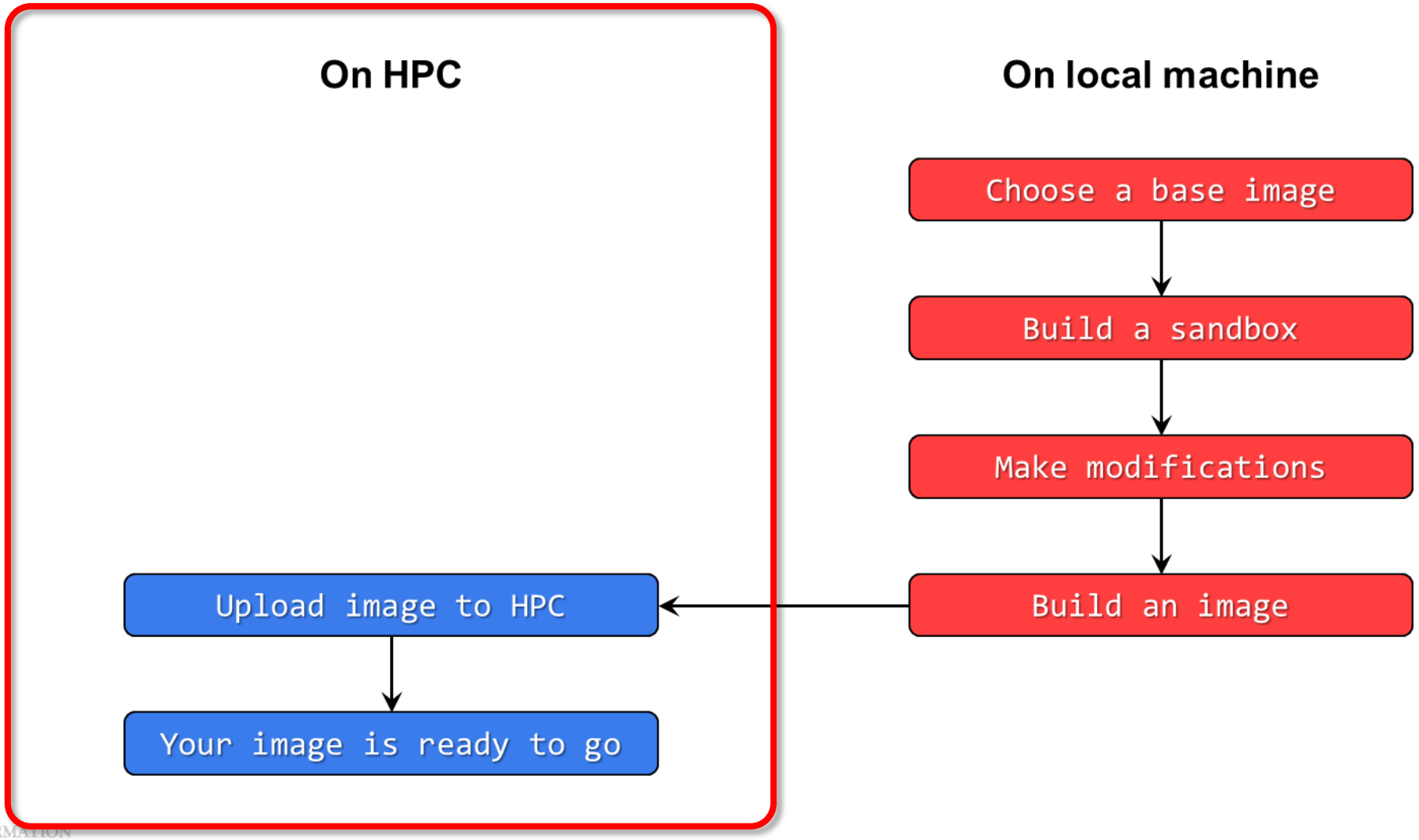
Summary


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

Summary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Conclusion

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Take home message

- **To use:**

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

- **To get:**

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

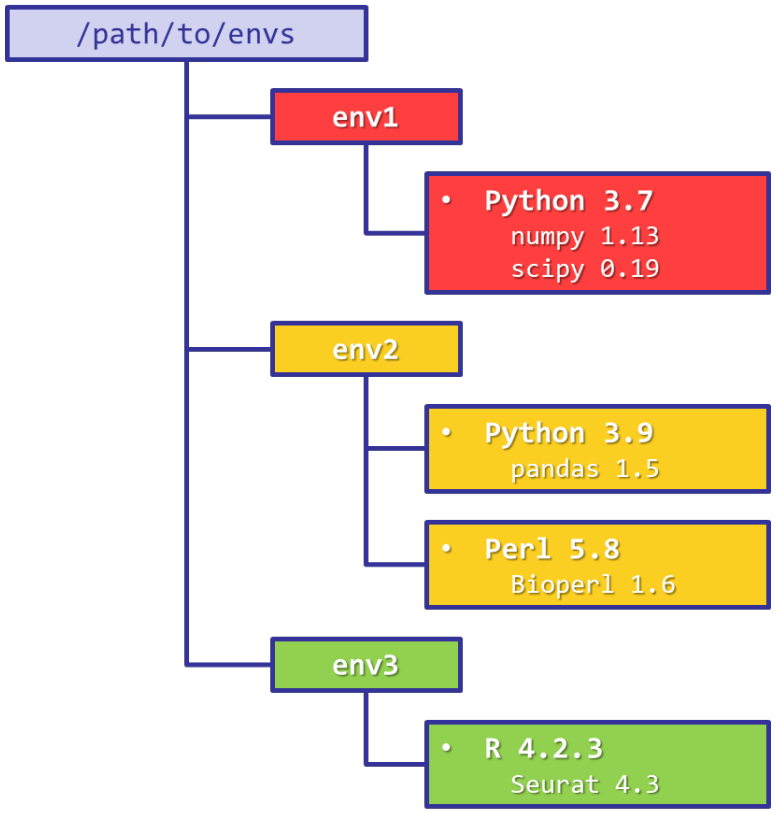
Contact us

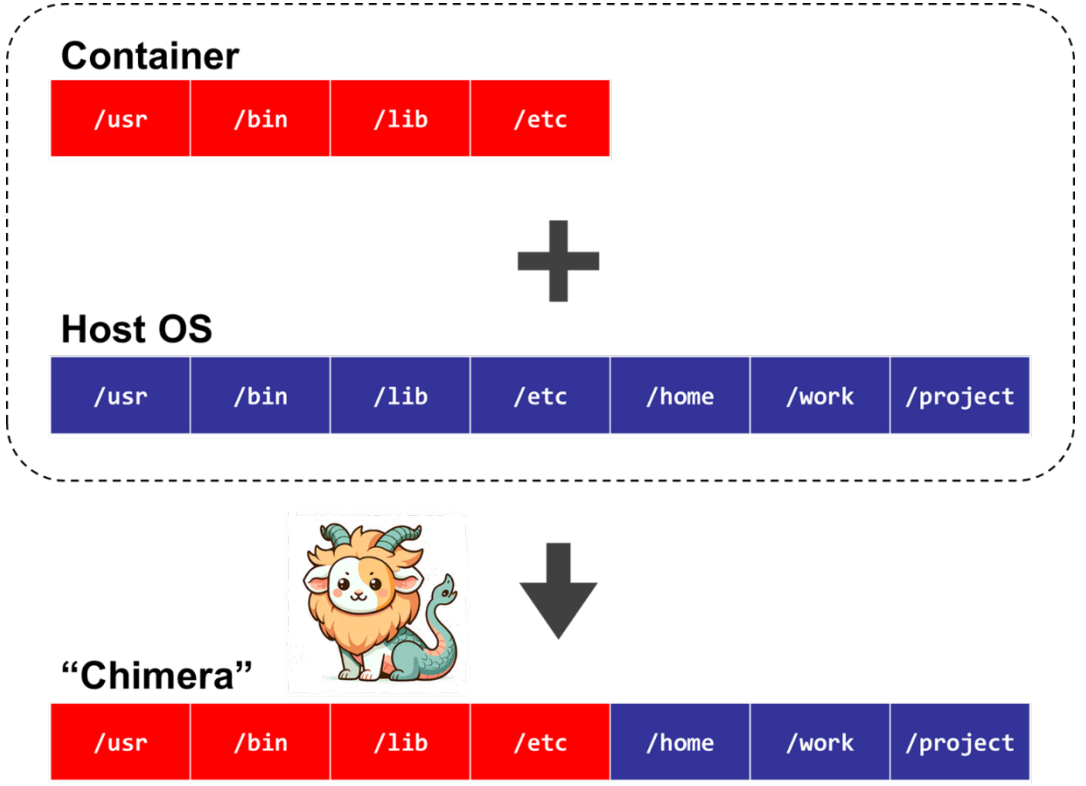
- **Contact user services**
  - Email Help Ticket: sys-help@loni.org
  - Telephone Help Desk: +1 (225) 578-0900

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 (but .yml may not work)	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

“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
```