Magic Tools To Install and Manage Software

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March 18, 2026

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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

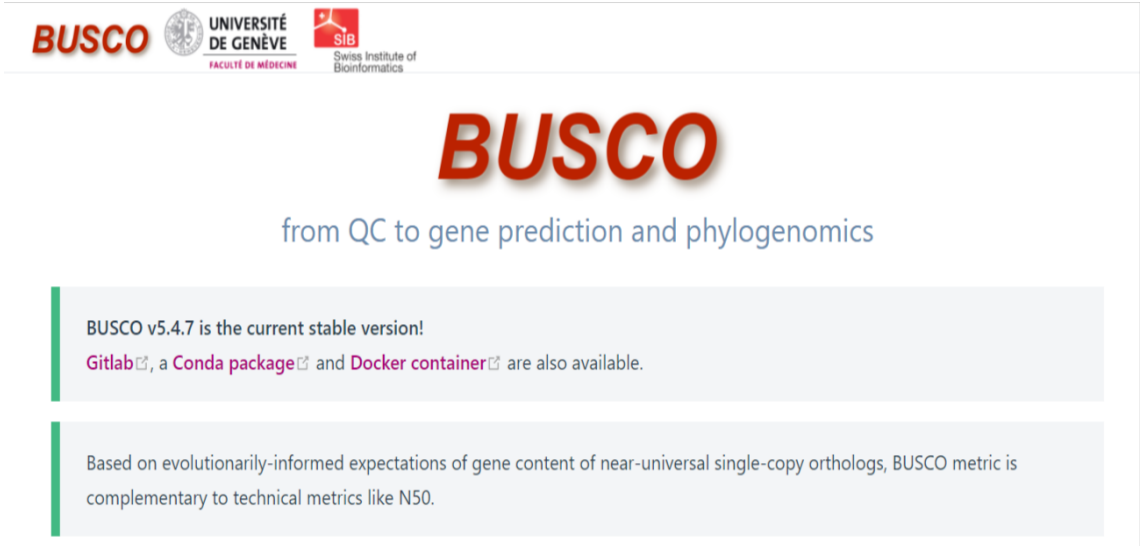
1

Dependencies

Most software depends on other libraries or tools. If those are missing, the software may not install or run.

1) Problems

1. **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/
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- https://ftp.ncbi.nlm.nih.gov/blast/executables/blast+/LATEST
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- 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.

LSU INFORMATION TECHNOLOGY SERVICES

1) Problems

1. **Dependencies** (Welcome to Linux!)

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- http://hmmer.org/
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> before attempting to run any BUSCO assessments.

- Dependencies

The following dependencies are required for AUGUSTUS:

- for gzip compressed input: (set ZIPINPUT = false in common.mk if … are not available)
  - libboost-iostreams-dev
  - zlib1g-dev
- for comparative AUGUSTUS (multi-species, CGP): (set COMPGENEPRED = false in … 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

1	**Dependencies** Most software depends on other libraries or tools. If those are missing, the software may not install or run.
2	**Version Conflicts** Different packages may need different versions of the same dependency, causing conflicts in a shared environment.

1) Problems

2) Conflicted packages

- Many scientific and ML applications require specific versions of Python, CUDA and libraries like TensorFlow, or PyTorch.
- For example:
  - TensorFlow 2.10 supports Python 3.7–3.10, not Python 3.11,
  - Combine with newer software in a working environment creates version conflicts.

1) Problems

1

Dependencies

Most software depends on other libraries or tools. If those are missing, the software may not install or run.

2

Version Conflicts

Different packages may need different versions of the same dependency, causing conflicts in a shared environment.

3

root permission

Installing software often requires admin access, which most HPC users do not have.

1) Problems

3) **Permission denied** (Welcome to HPC!)

```
[kasetti@mike003 E3RC]$ module load python
[kasetti@mike003 E3RC]$ pip install gdal
```

1) Problems

3) **Permission denied** (Welcome to HPC!)

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[kasetti@mike003 E3RC]$ module load python
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```

```
  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 92, in fetch_config
    File "/usr/local/packages/python/3.9.7-anaconda/lib/python3.9/subprocess.py", line 951, in __init__
      self._execute_child(args, executable, preexec_fn, close_fds,
    File "/usr/local/packages/python/3.9.7-anaconda/lib/python3.9/subprocess.py", line 1821, in _execute_chi
ld
      raise child_exception_type(errno_num, err_msg, err_filename)
  FileNotFoundError: [Errno 2] No such file or directory: 'gdal-config'
```

1) Problems

3) **Permission denied** (Welcome to HPC!)

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[kasetti@mike003 E3RC]$ module load python
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```
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```

libgdal

1) Problems

3) **Permission denied** (Welcome to HPC!)

- If you ask Google / ChatGPT…

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

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

1) Problems

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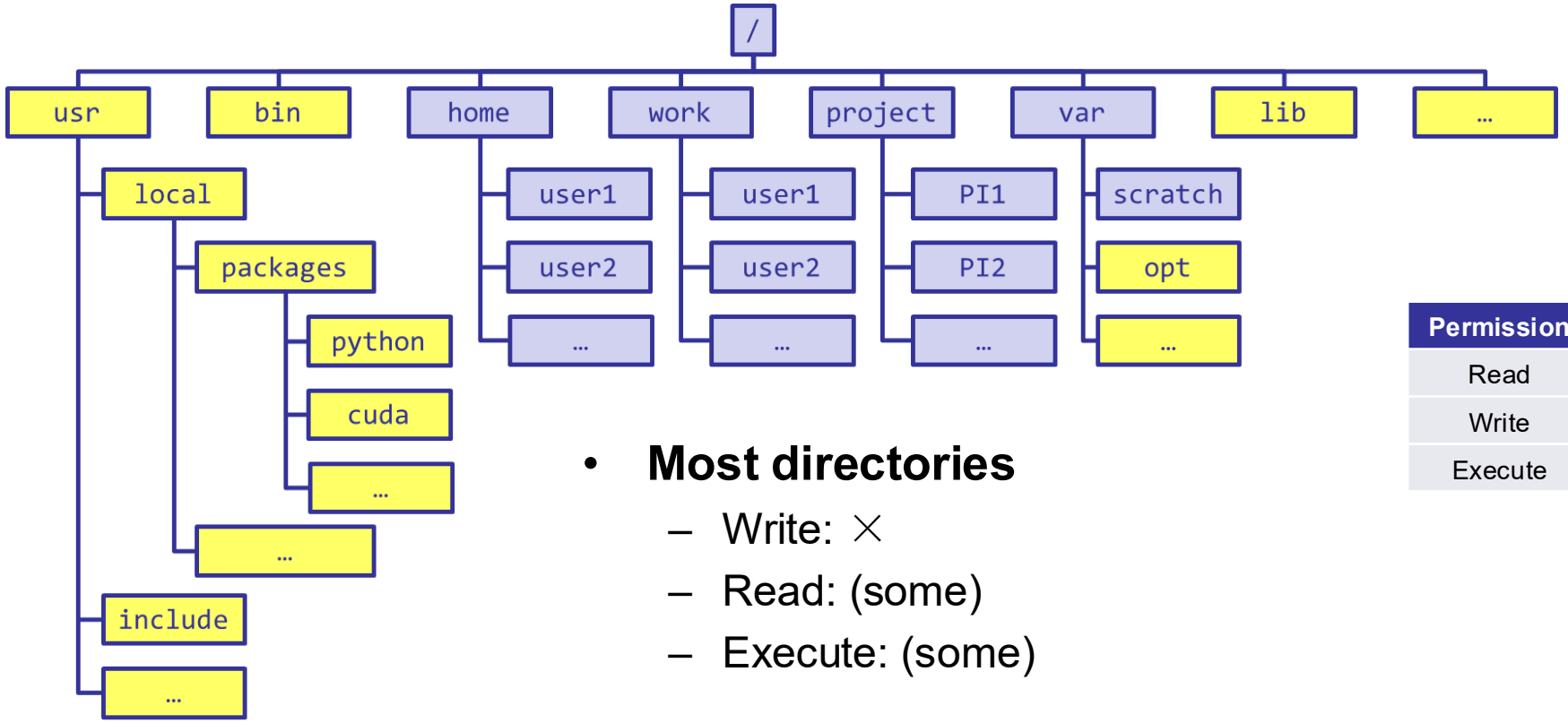

Permission			
Read	√	×	√*
Write	√	×	×
Execute	√	×	√*

- **Most directories**
  - Write: ×
  - Read: (some)
  - Execute: (some)

1) Problems

1

Dependencies

Most software depends on other libraries or tools. If those are missing, the software may not install or run.

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4

Reproducibility

Reproducing the same setup or sharing it with others can be surprisingly difficult.

4. Reproducibility - 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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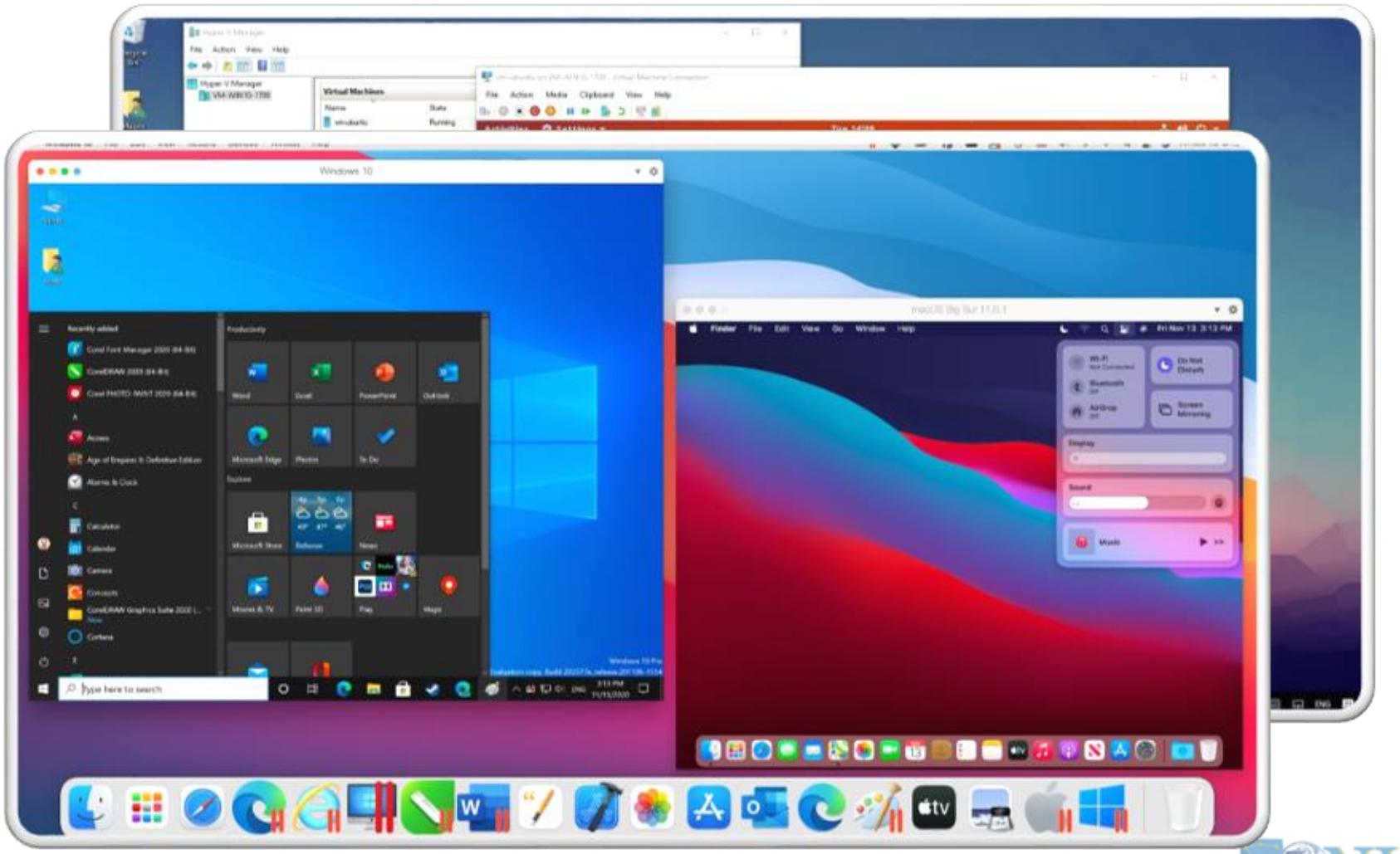
2) Container & Singularity

a) What is a container?

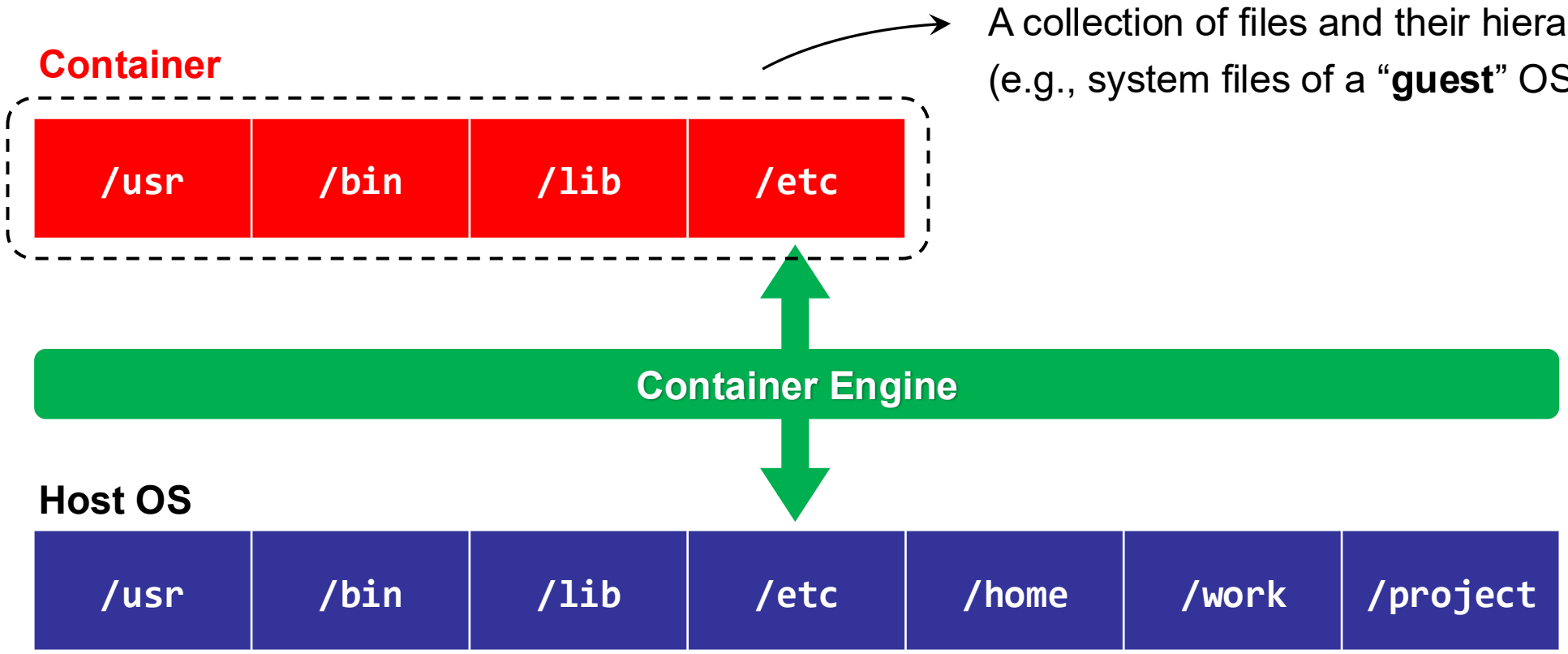
- **Virtual machine**
  - "Virtualize" / "mimic" an **entire computer** on another computer
  - Virtualize both **hardware** and **software**



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?



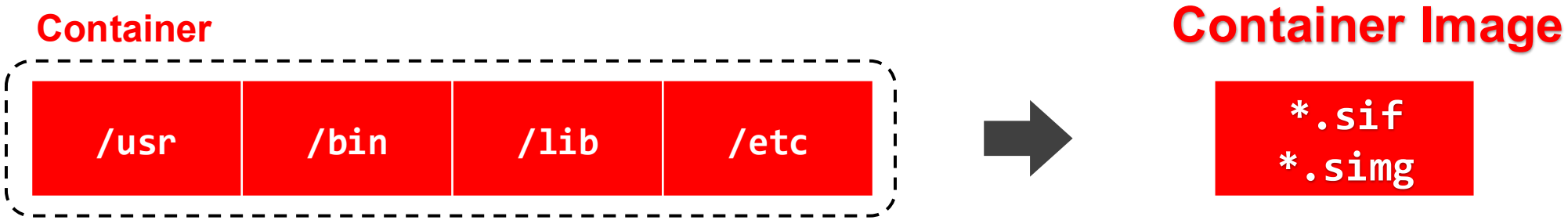
a) What is a container?

/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

2) Container & Singularity

a) What is a container?

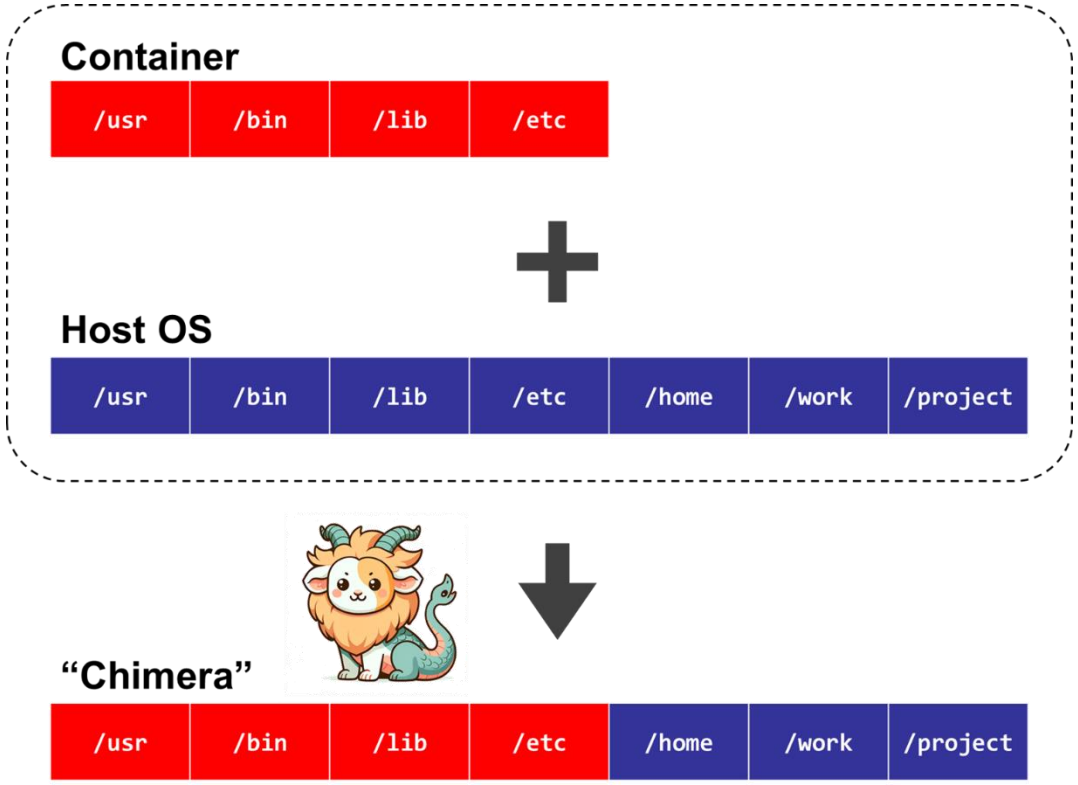


a) What is a container?

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

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

    Whatever happens in a container stays in that container…



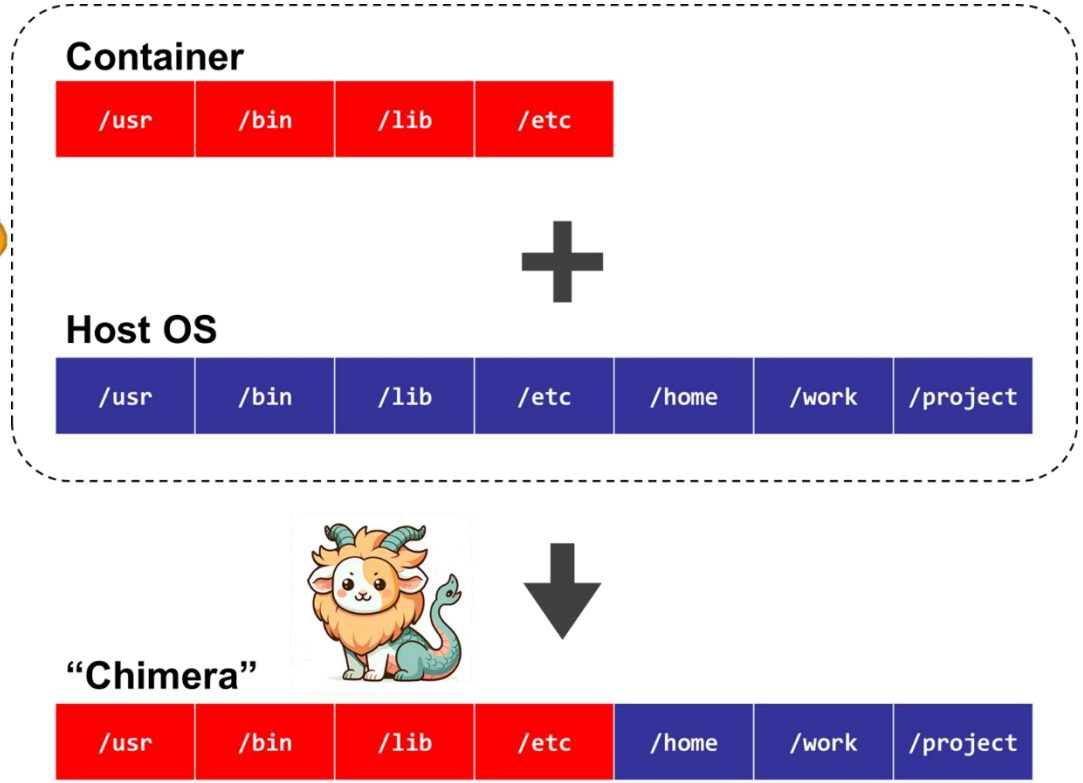
b) How does it solve my problems?

- **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

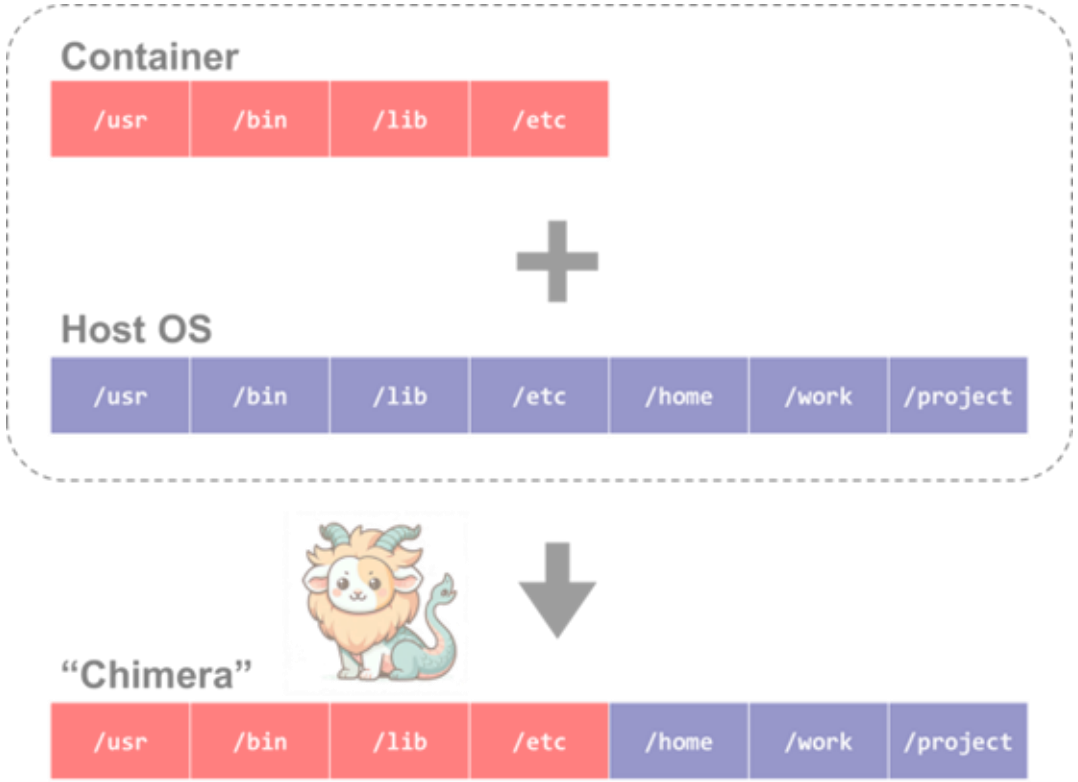
- **Conflicted packages**
  - Install in different containers.

- **Share / Migrate**
  - Copy-paste a container image!



c) What is Singularity?

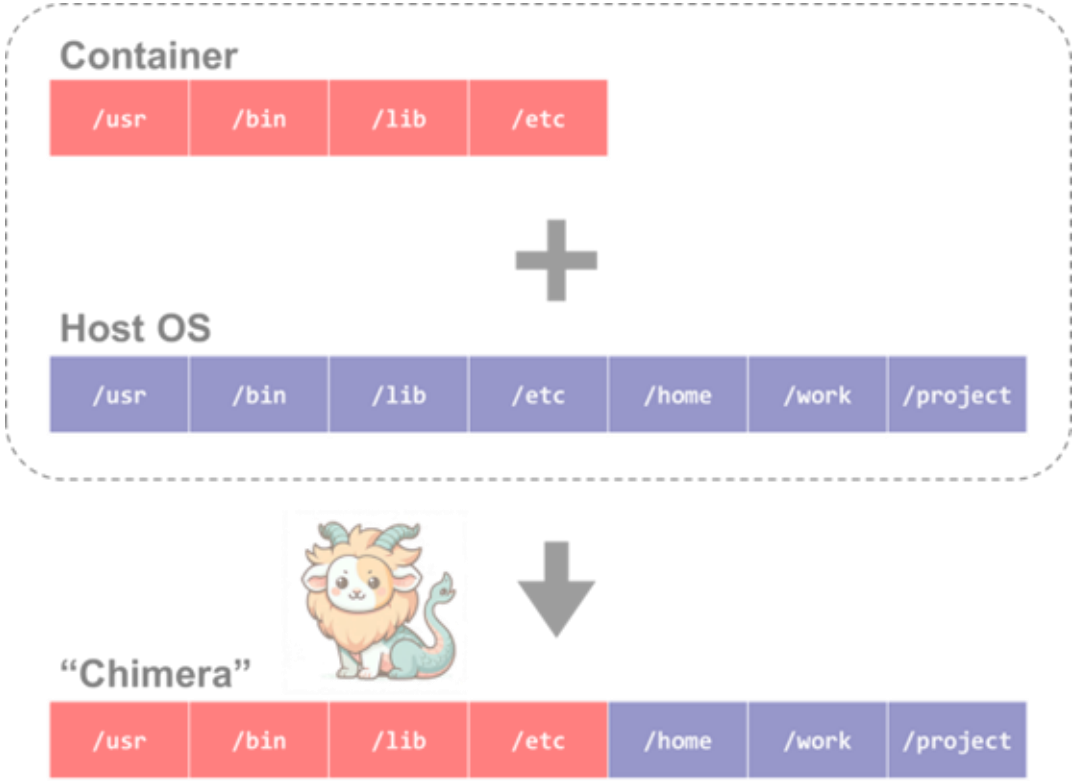
Technology →



c) What is Singularity?

Singularity

↑ **Software** system that implements the technology



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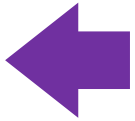
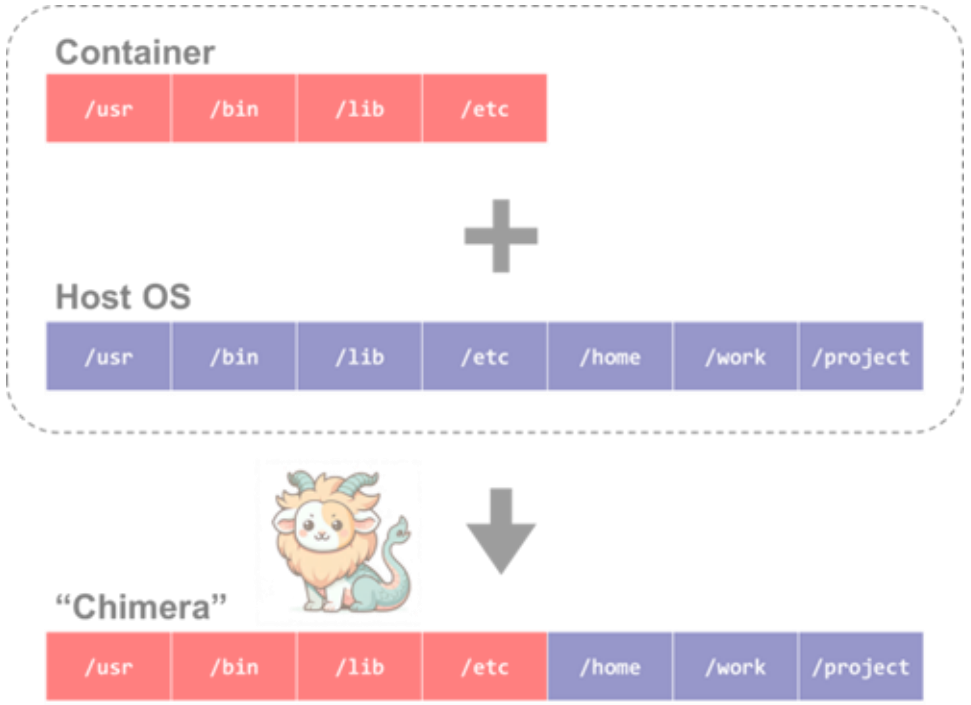


- Does **NOT** need root privileges
- "**Container for HPC**"

- **Needs** root privileges

Summary



Technology that helps with software installation

Software system that implements the technology

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Basic Information

- **Singularity availability**

a) On **all clusters**

- ✓ **LSU HPC**: SMIC, Deep Bayou, SuperMike 3
- ✓ **LONI**: QB3, QB4

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

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2) Basic commands

- **Available images**

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

```
[kasetti@qbd1 ~]$ ls /project/containers/images/
adcirc.5bc04d6.centos8.sif                  mesos_1.9.0_ubuntu16.04.simg
adcirc.5bc04d6.rky8.5.sif                   minknow22.sif
adcirc.5bc04d6.sif                          nco-4.9.8.sif
agat-1.4.0.sif                              nextflow-23.10.1.sif
alphafold-catgumag-2.2.sif                  nvidia-dli.sif
alps-2.3.0-dockerhub.simg                   octopus-14.0.sif
alps-2.3.0-dockerhub-v2.simg                ollamaondemand-1.0.0.sif
bcftools-1.18.sif                           ollamaondemand-1.0.0.sif.old
beast2-2.7.7.sif                            openbabel-3.1.1.sif
blast-2.14.1.sif                            openfoam10-openmpi.4.0.3-pmi2.sif
blender-2.79b-cuda-8.0-ubuntu-16.04.simg    openfoam9.sdfibm-openmpi.4.0.3-pmi2.sif
bowtie2-2.5.1.sif                           openfoam-v2212-openmpi.4.1.2-pmi2.sif
braker-3.0.8.sif                            openfoam.v9.sdfibm.sif
busco-5.7.1.sif                             paraviewweb-5.12.1.sif
```

2) Basic commands

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

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

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

2) Basic commands

a) Common usage 1: Open a 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) • Access host files with bind mounts • /home, /work 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: `/project/containers/images/singularity-training-ubuntu.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

2) Basic commands

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>`	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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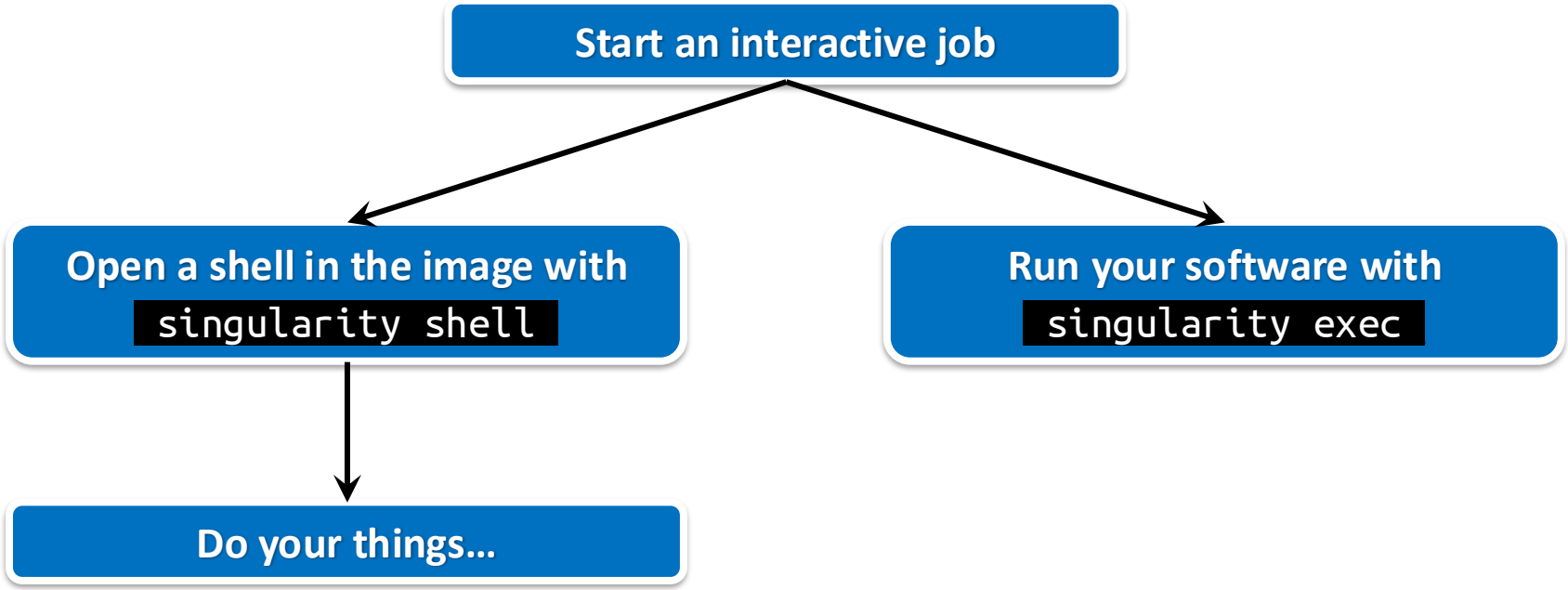
3) Run jobs with Singularity

- **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

```
#!/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/singularity-
training-ubuntu.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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3. Get More Container Images

- **Available images**

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

```
[kasetti@qbd1 ~]$ ls /project/containers/images/
adcirc.5bc04d6.centos8.sif                  mesos_1.9.0_ubuntu16.04.simg
adcirc.5bc04d6.rky8.5.sif                   minknow22.sif
adcirc.5bc04d6.sif                          nco-4.9.8.sif
agat-1.4.0.sif                              nextflow-23.10.1.sif
alphafold-catgumag-2.2.sif                  nvidia-dli.sif
alps-2.3.0-dockerhub.simg                   octopus-14.0.sif
alps-2.3.0-dockerhub-v2.simg                ollamaondemand-1.0.0.sif
bcftools-1.18.sif                           ollamaondemand-1.0.0.sif.old
beast2-2.7.7.sif                            openbabel-3.1.1.sif
blast-2.14.1.sif                            openfoam10-openmpi.4.0.3-pmi2.sif
blender-2.79b-cuda-8.0-ubuntu-16.04.simg    openfoam9.sdfibm-openmpi.4.0.3-pmi2.sif
bowtie2-2.5.1.sif                           openfoam-v2212-openmpi.4.1.2-pmi2.sif
braker-3.0.8.sif                            openfoam.v9.sdfibm.sif
busco-5.7.1.sif                             paraviewweb-5.12.1.sif
```

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   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

1) What you need

BEFORE

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

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

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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 !**

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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

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/ • **BUT!** Do **NOT** 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

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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

- **BONUS: Hot packages!**

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

```
$ singularity pull docker://pytorch/pytorch:2.10.0-cuda13.0-cudnn9-devel
```

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

```
$ singularity pull docker://tensorflow/tensorflow:2.21.0-gpu-jupyter
```

3) How to get

- **BONUS: Hot packages!**

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

```
$ module load pytorch
```

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

```
$ module load tensorflow
```

Summary

- **Pull the image or/and build the image**

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

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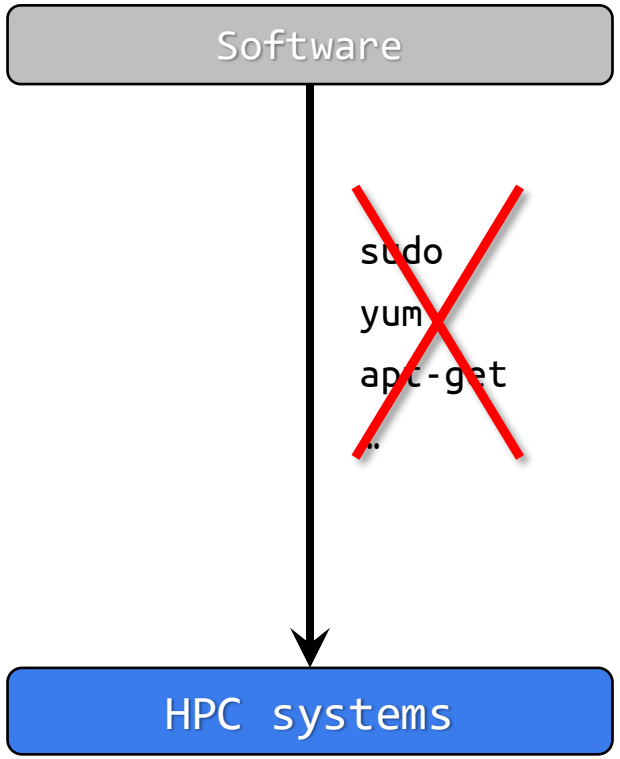
4. Build Your Own Container Image

- **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).

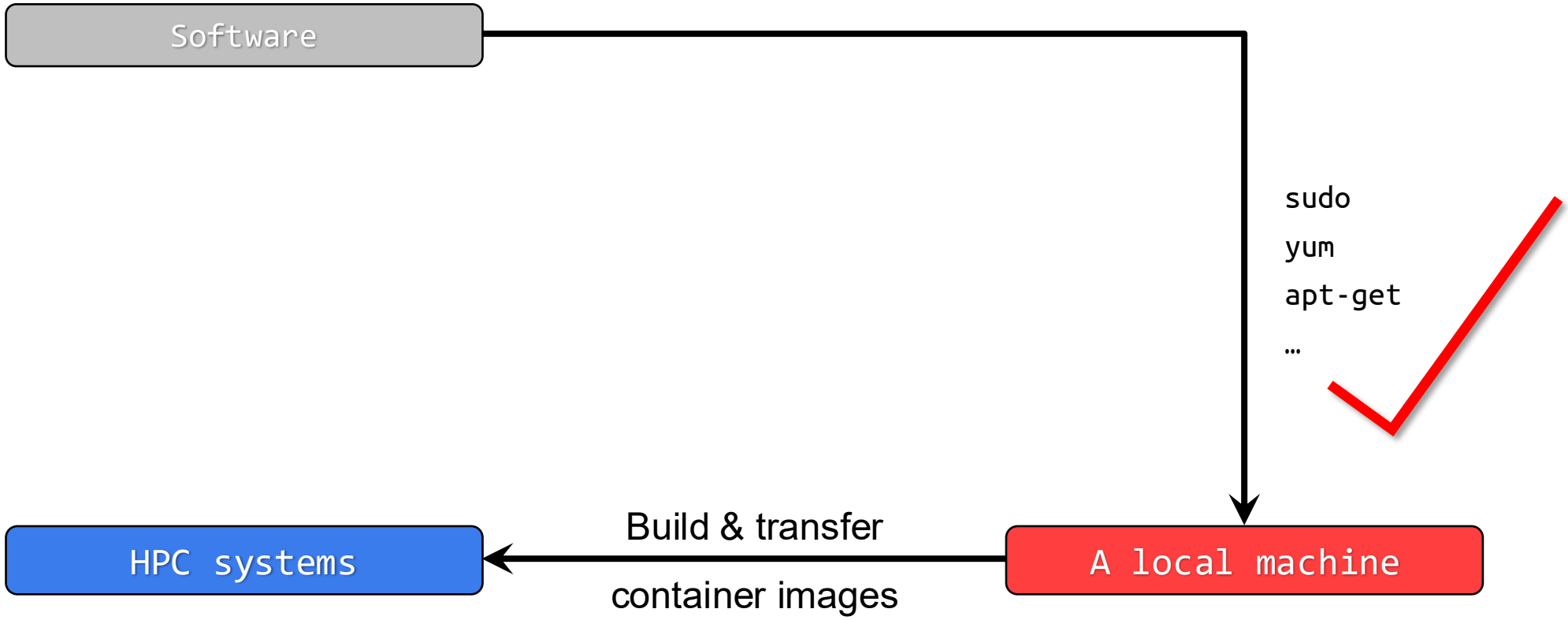
4. Build Your Own Container Image

- **Idea**



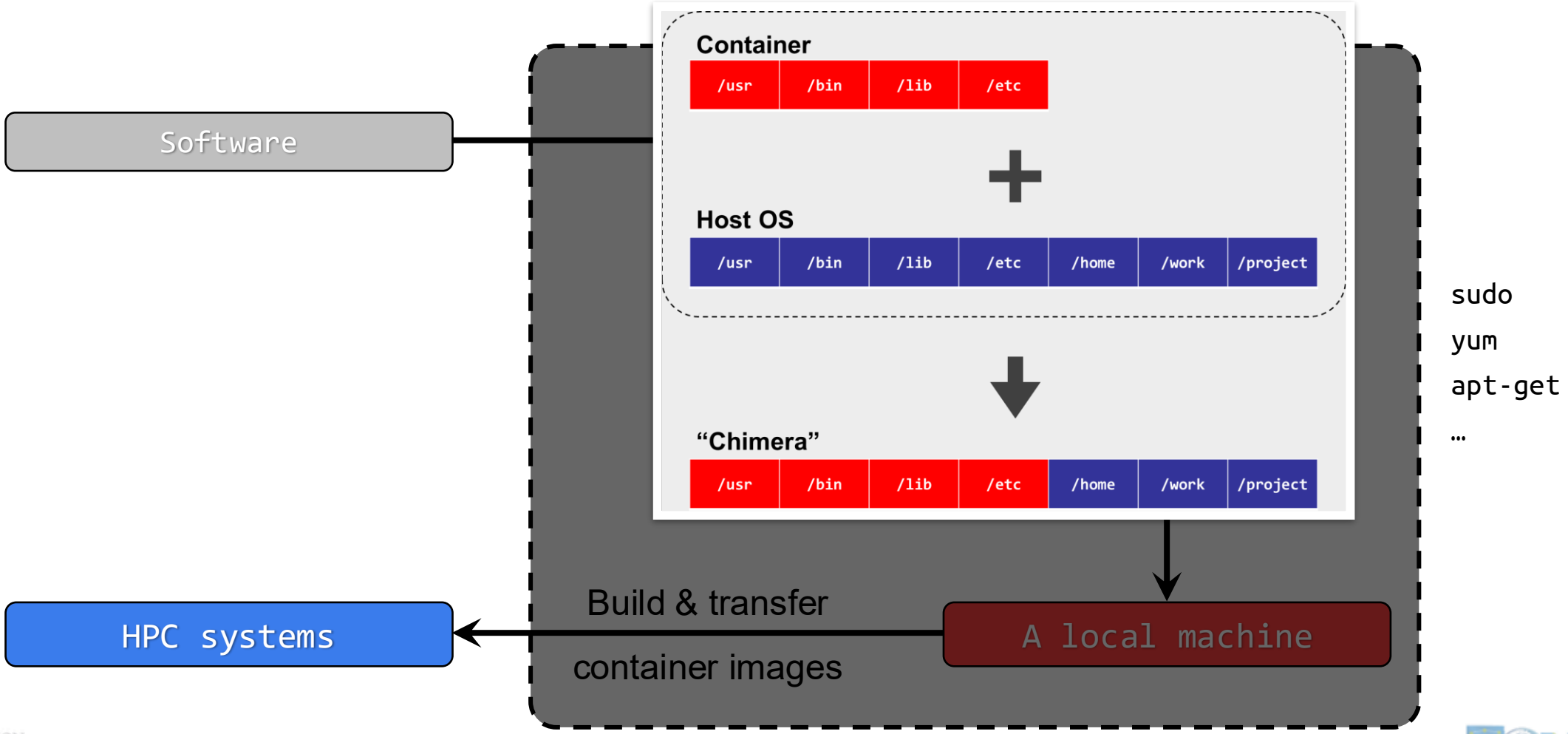
4. Build Your Own Container Image

- **Idea**



4. Build Your Own Container Image

- **Idea**



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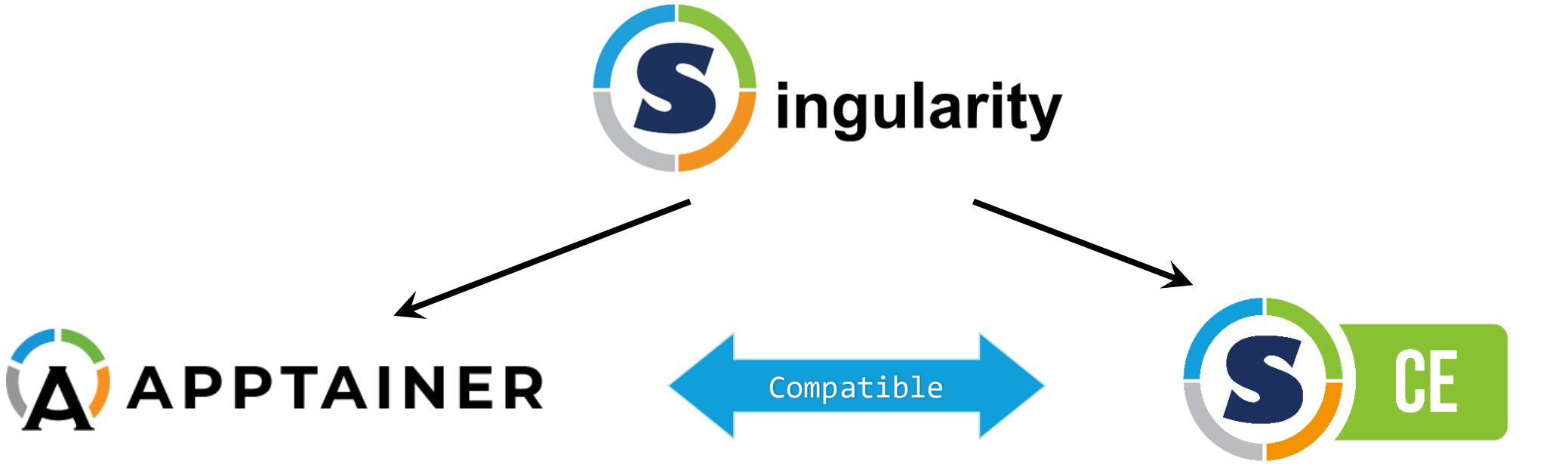
1) What you need

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**

- **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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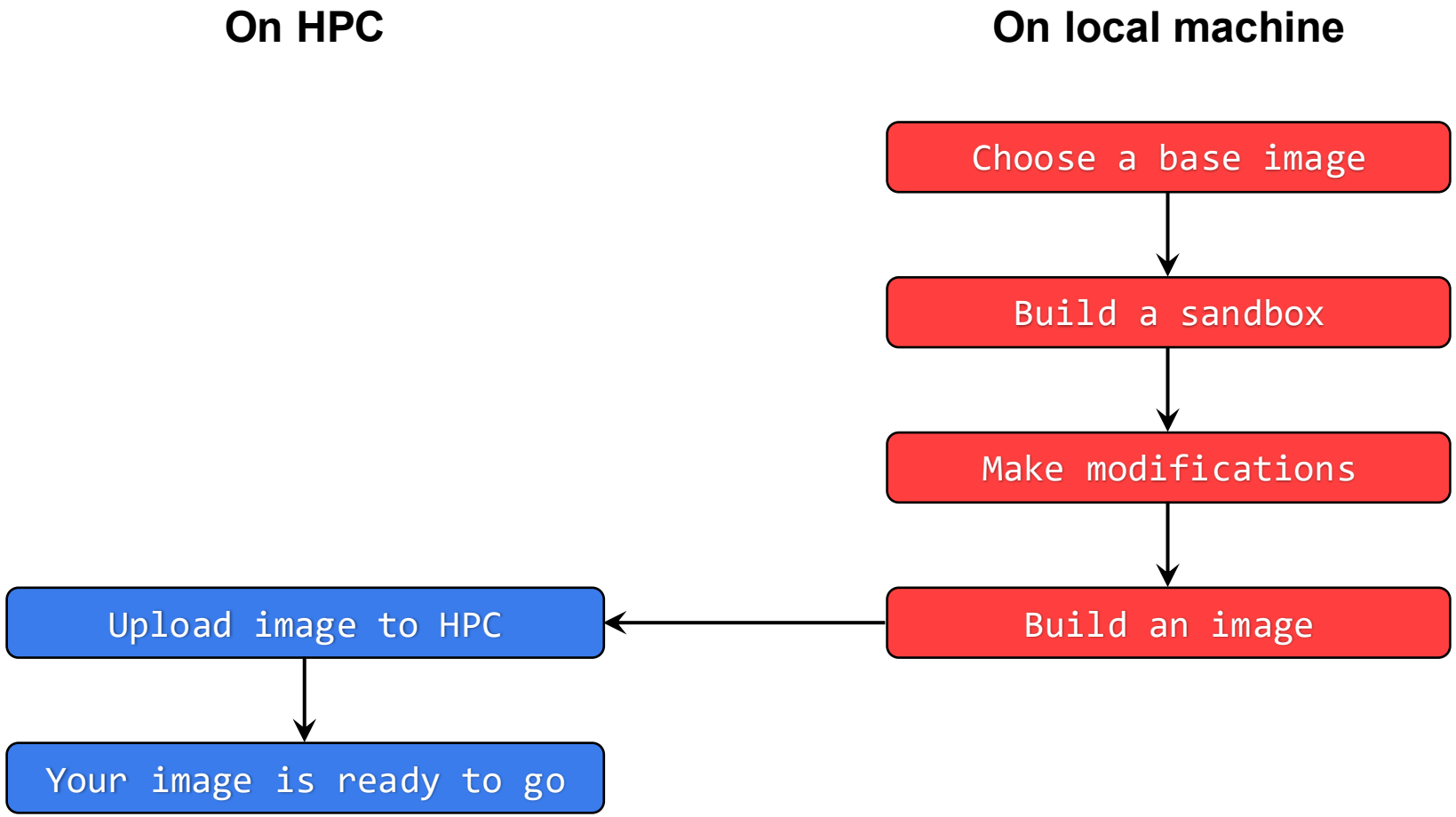
2) Typical workflow



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

   – Read-only without it

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

- Read-only without it

2) Typical workflow

c) Make modifications

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

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

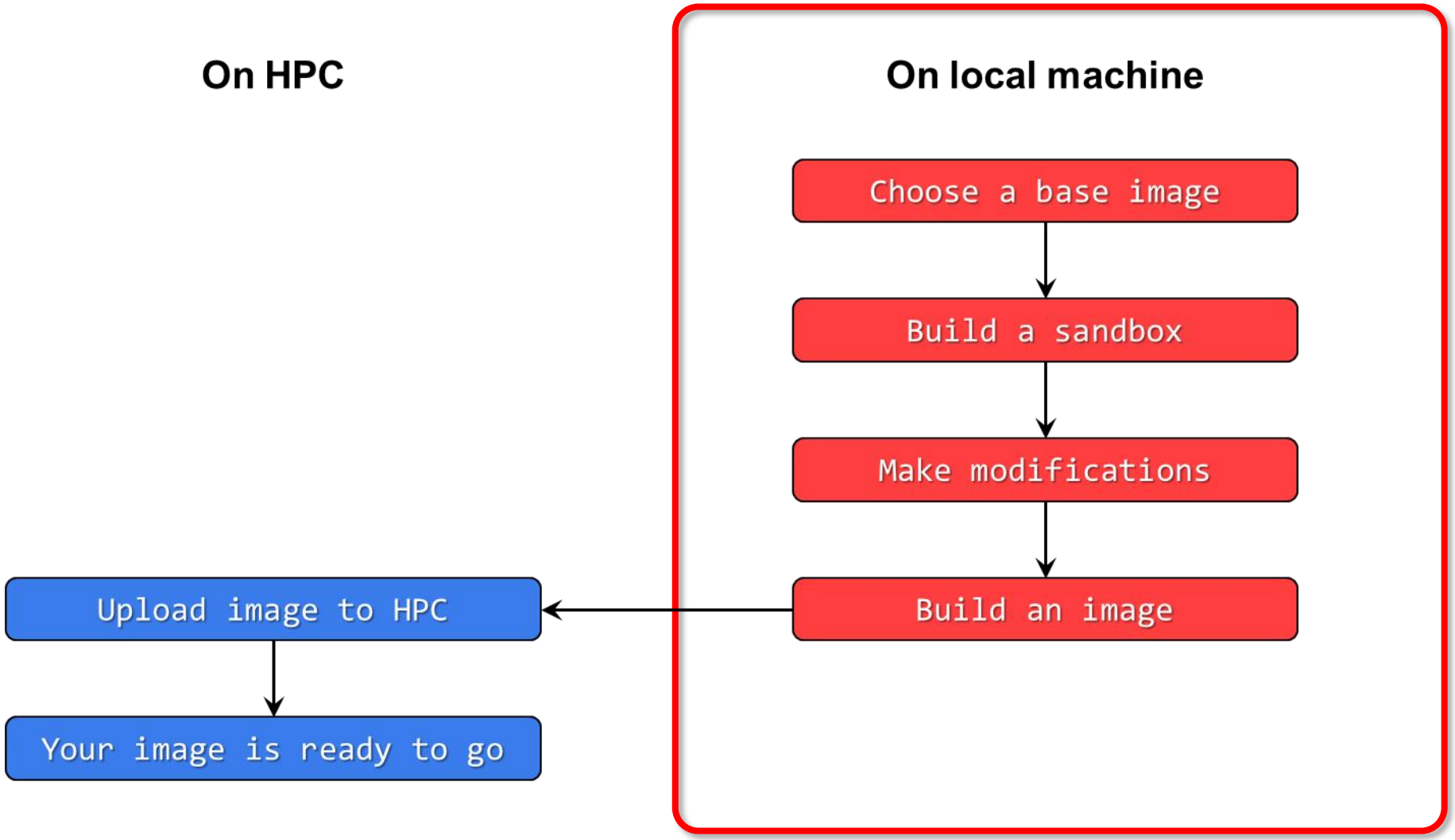
- **Quick recap**

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 ...`

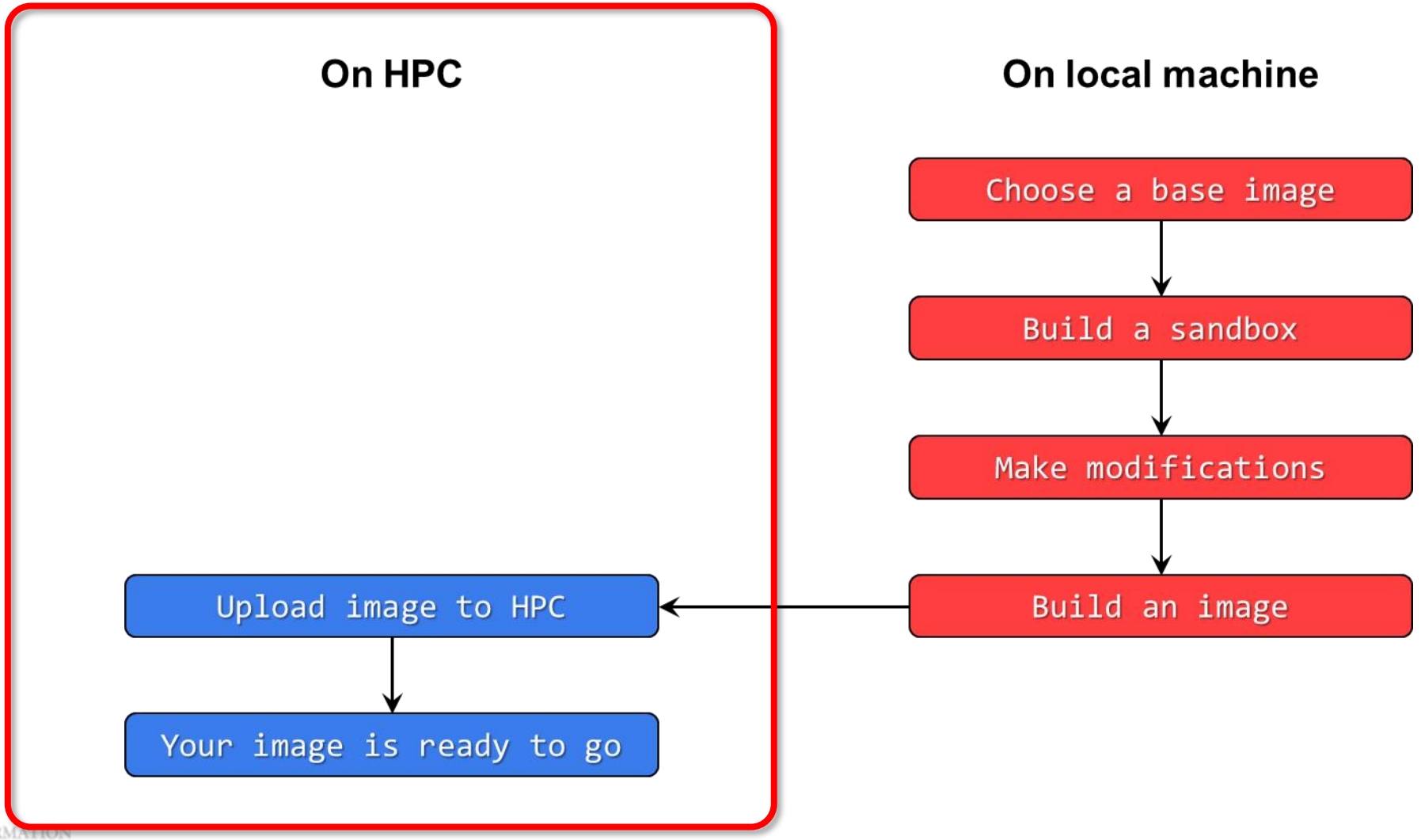
e) Upload image to HPC and run

Now! The moment of truth!

2) Typical workflow



2) Typical workflow



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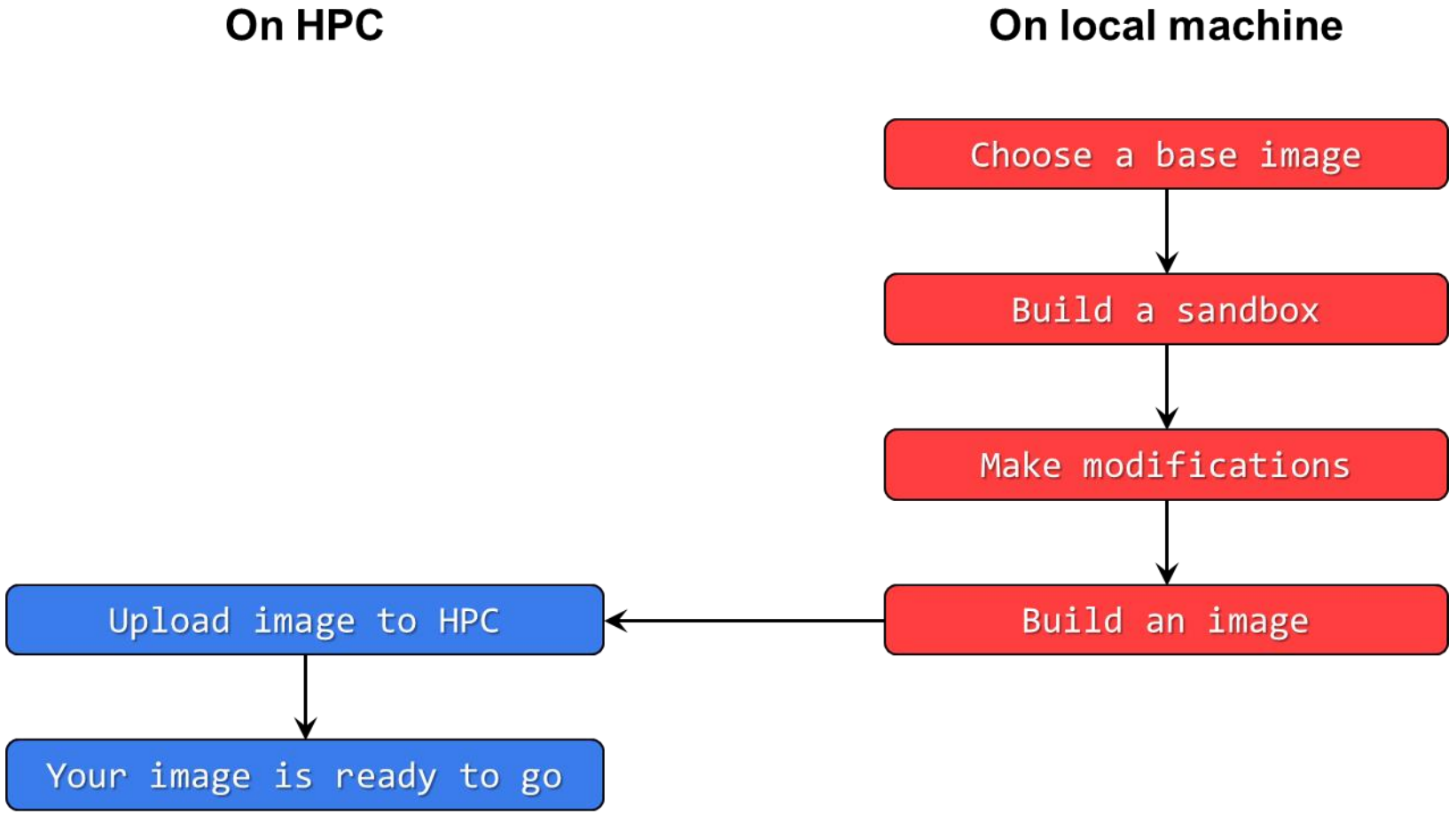
3) Make it easier - Recipe

- **Why?**



3) Make it easier - Recipe

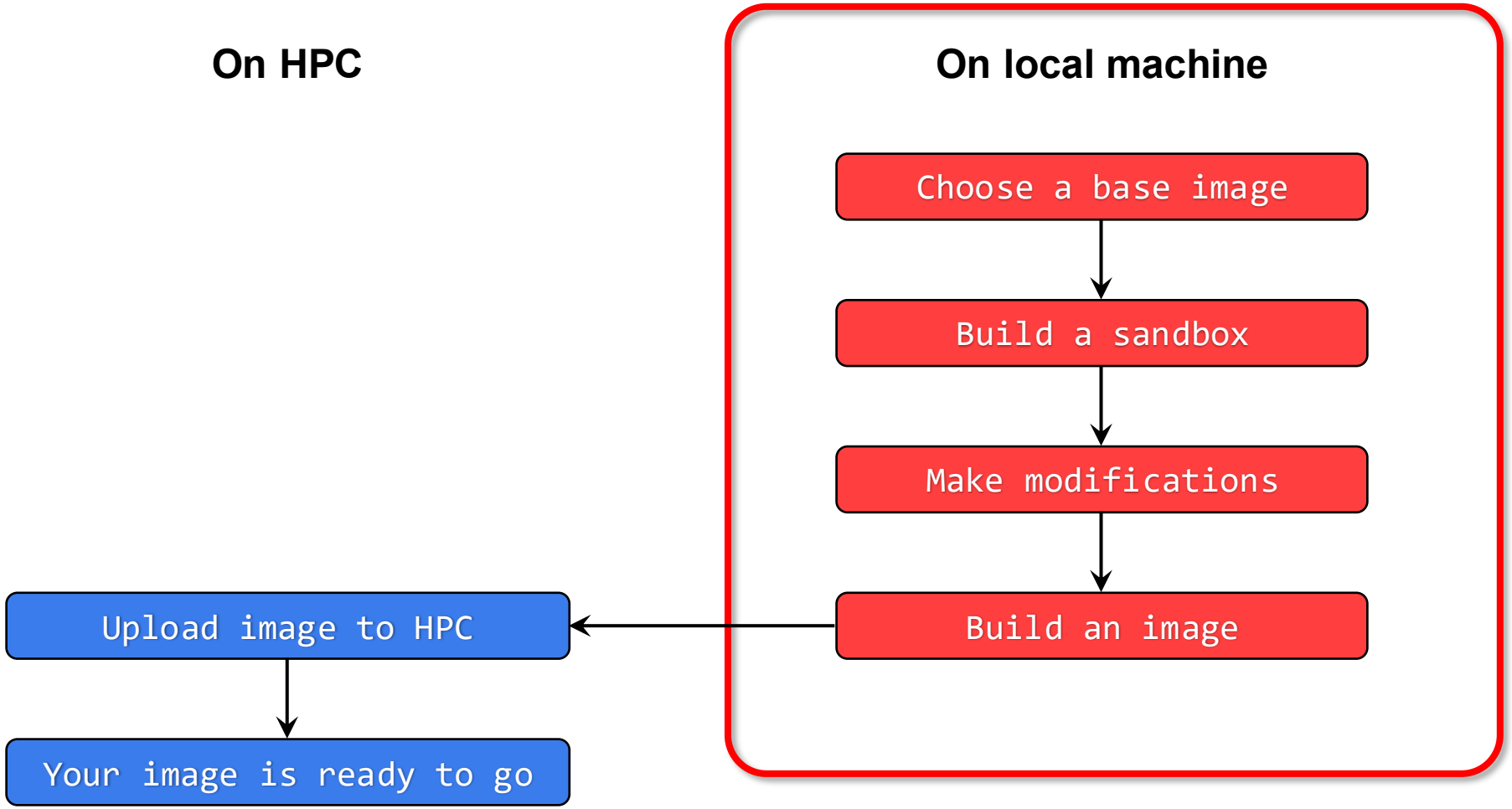
- **Why?**

Pros	Cons
• Flexibility	• Repeatability • Minimizing image size

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

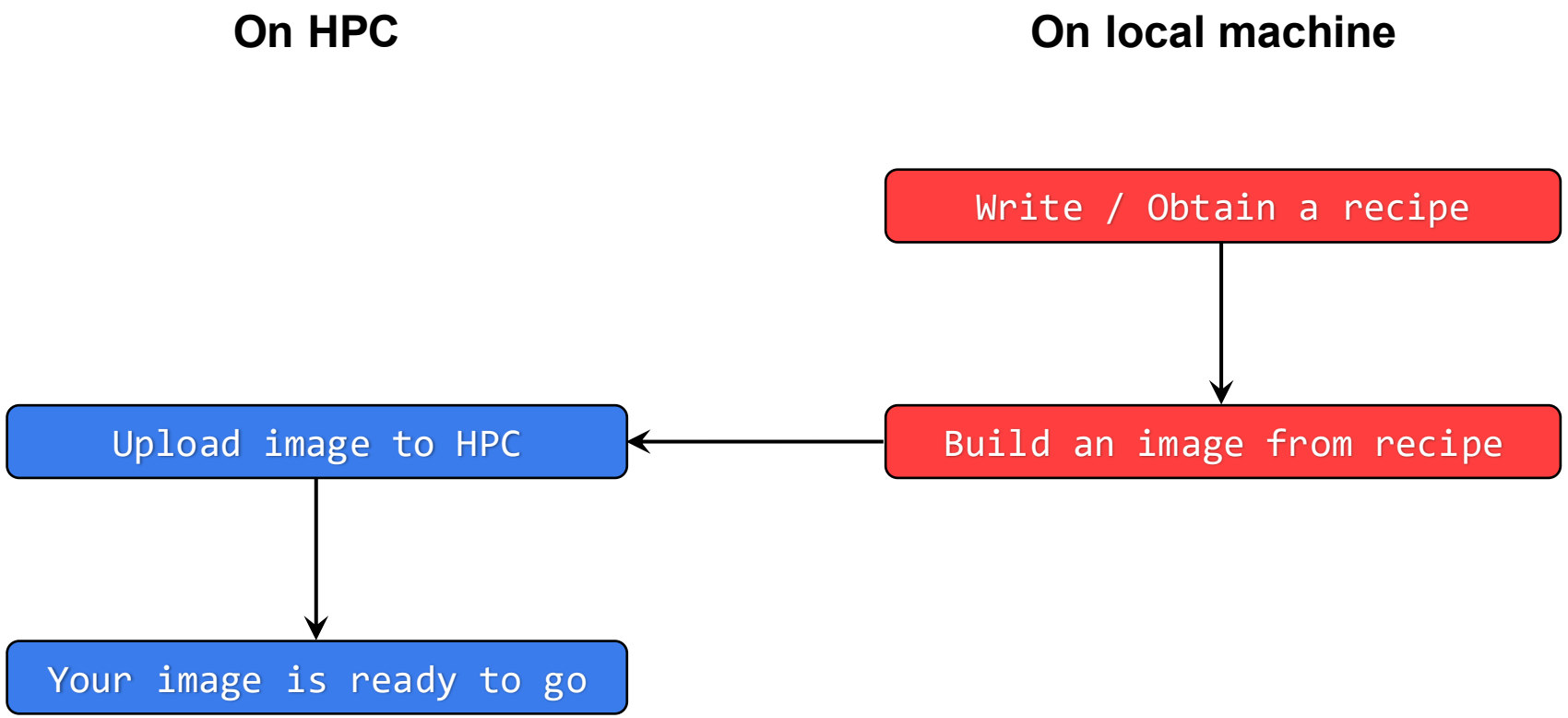
3) Make it easier - Recipe

- **Why?**



3) Make it easier - Recipe

- **Why?**



3) Make it easier - Recipe

a) What does a recipe look like?

recipe.def

```
Bootstrap: docker
From: ubuntu:24.04

%labels
    Author Siva Prasad Kasetti
    Version 1.0
    Description Install curl

%post
    apt-get update -y
    apt-get install -y curl

%environment
   export MYENV="This is my environment variable."

%runscript
   echo "Print curl verson:"
   curl --version
```

3) Make it easier - Recipe

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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`

3) Make it easier - Recipe

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3) Make it easier - Recipe

b) Build the recipe

```
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```

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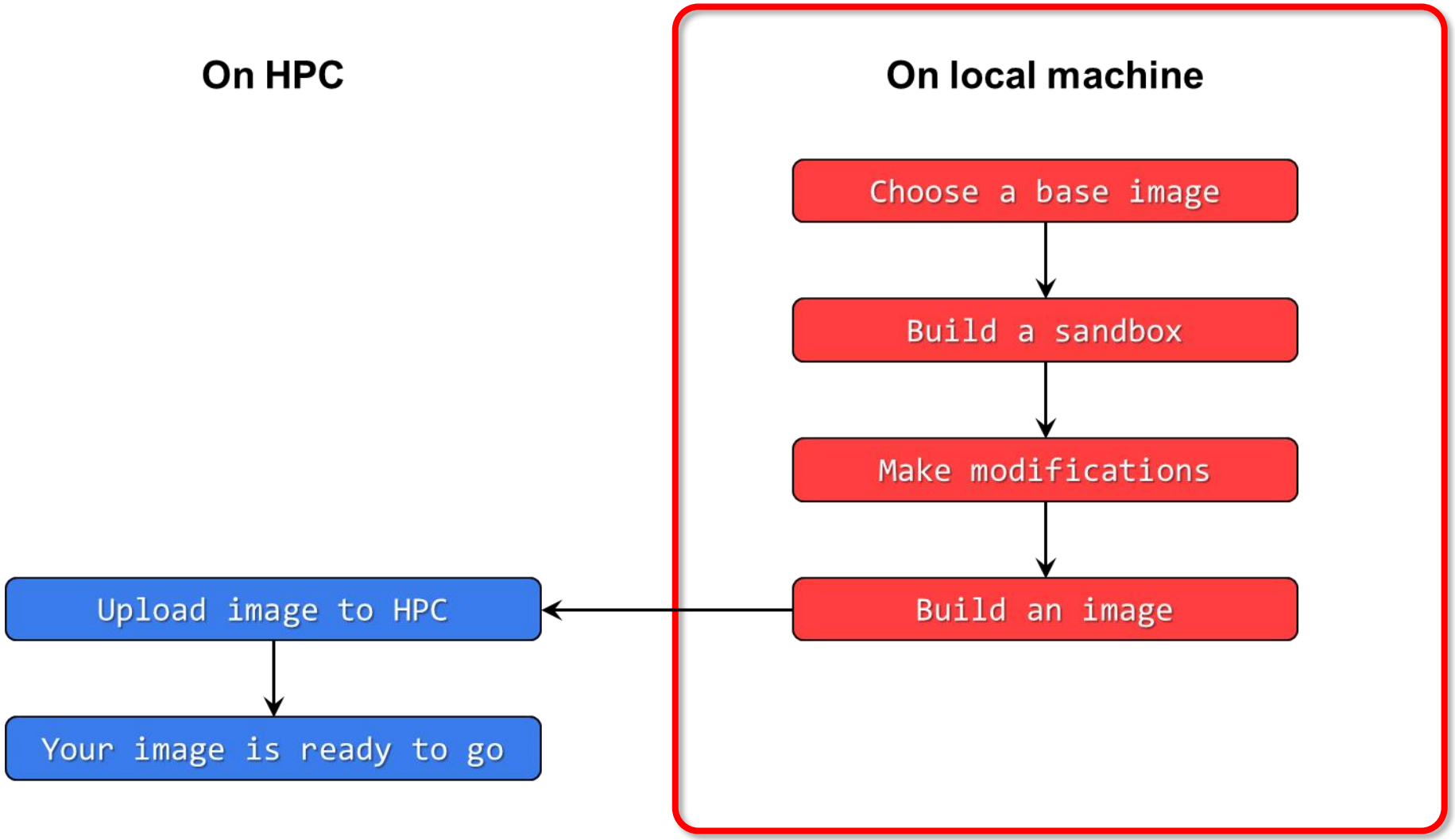
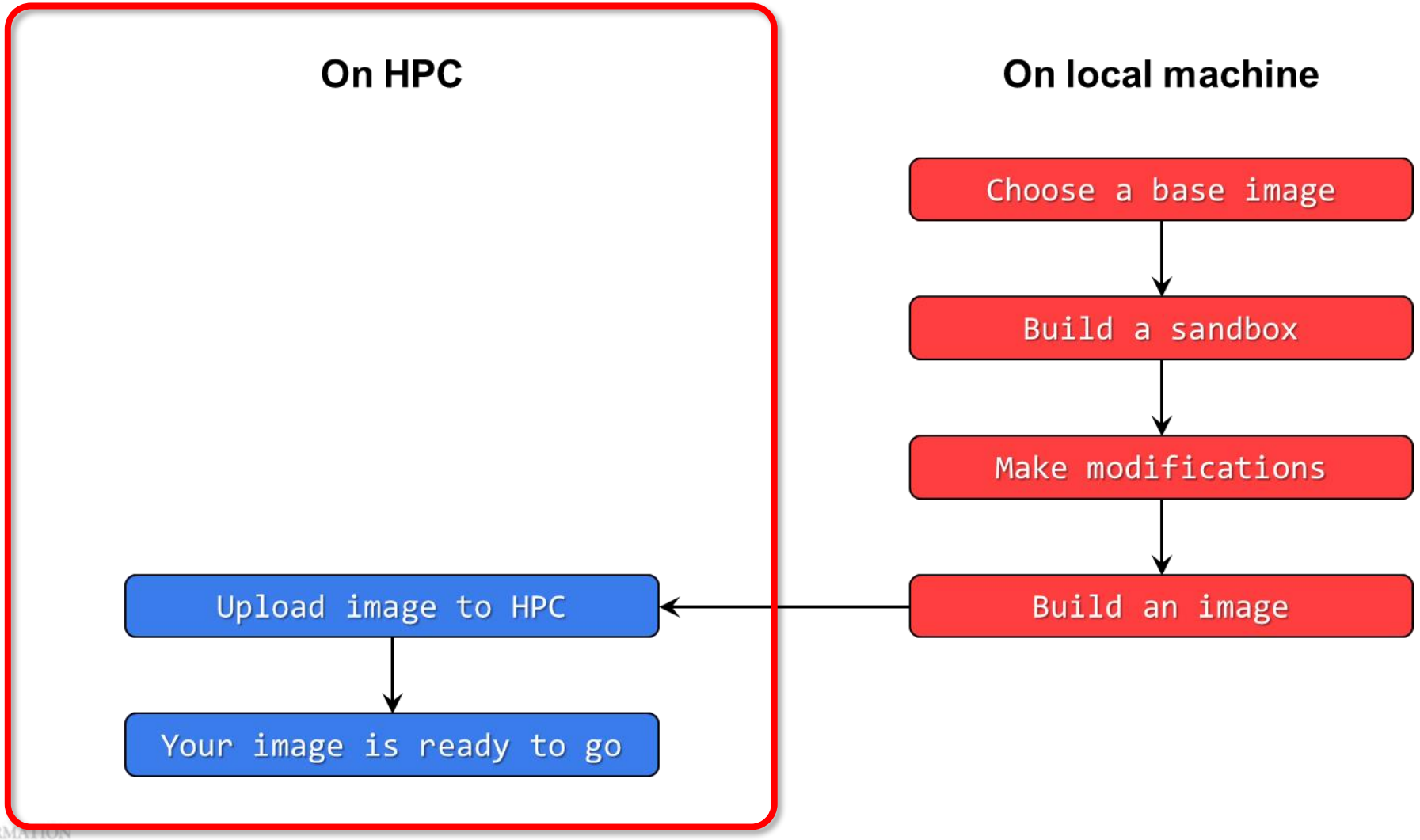
Summary


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

Conclusion

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   1) Problems
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2. **Run an Existing Container Image**
   1) What you need
   2) Basic commands
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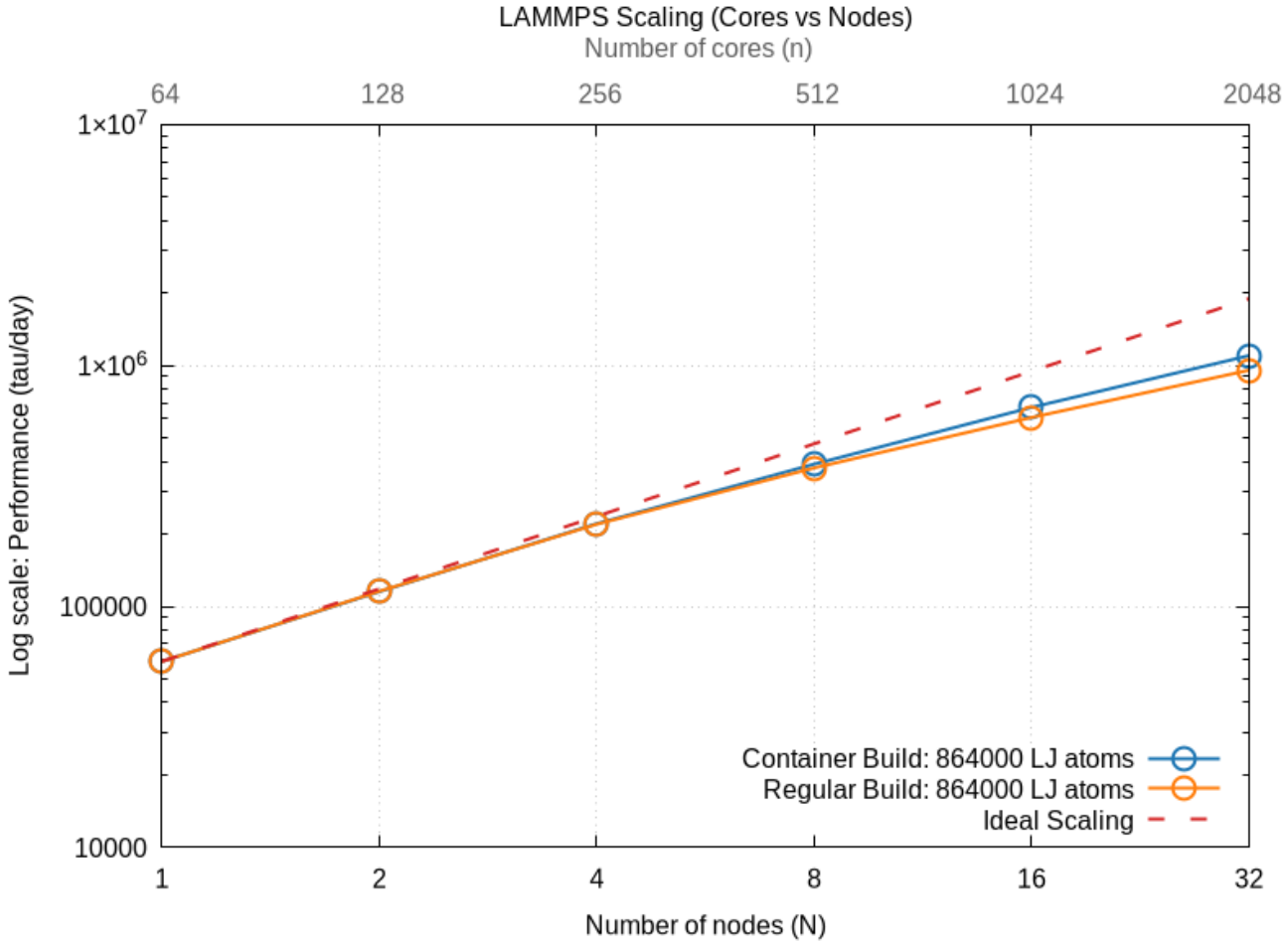
Performance Comparison

- The MD simulation package **LAMMPS** was used as the benchmark.
- Performance was compared between running LAMMPS directly from source and running it inside a container.
- Results showed identical performance between both approaches.



Contact us

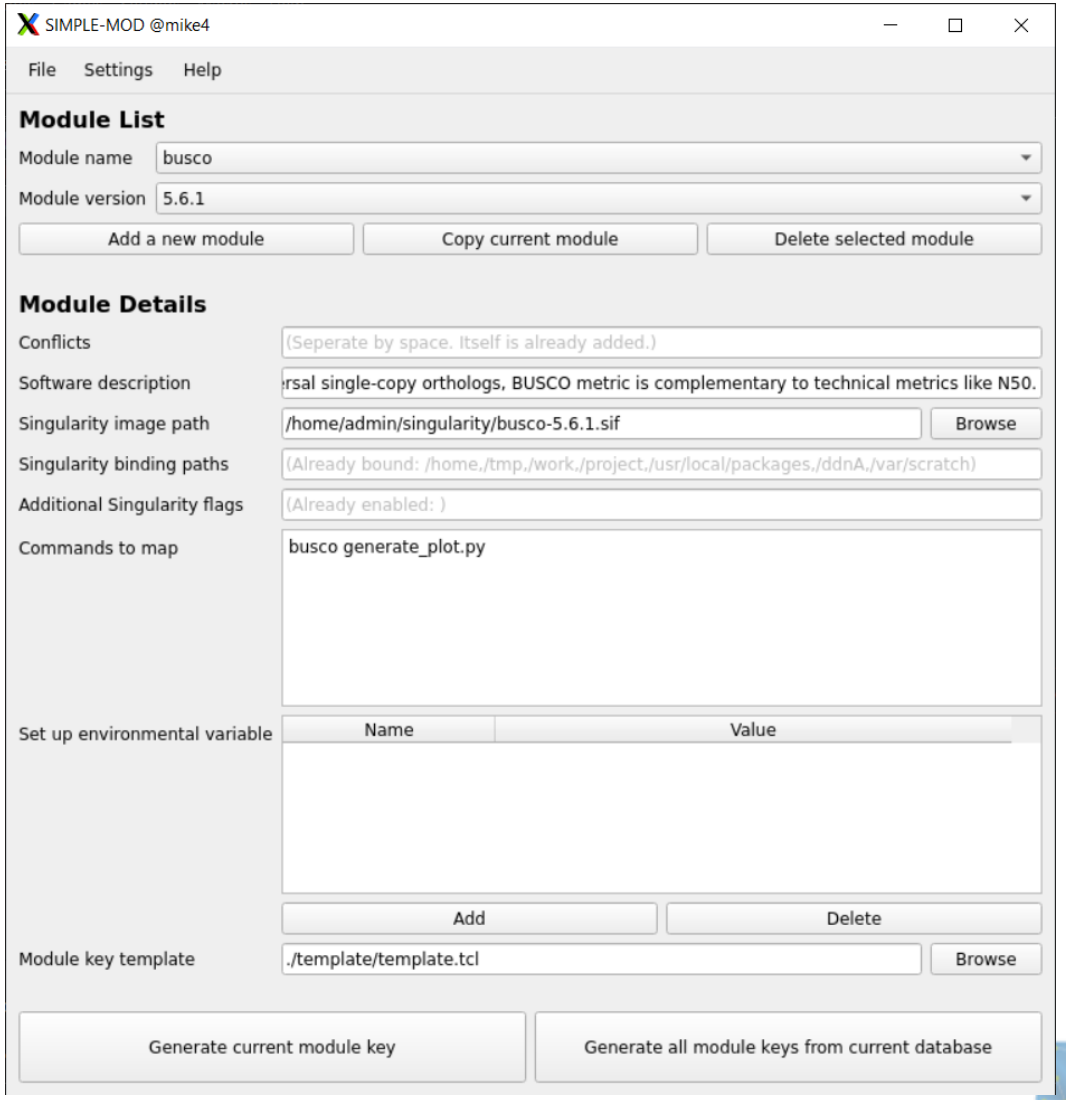
- **Contact user services**
  - Email Help Ticket: sys-help@loni.org
  - Telephone Help Desk: +1 (225) 578-0900

“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
```