Apptainer Containers for HPC systems

We'll look at...

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1. Introduction to Containers for HPCs
2. Cluster admins and container tech
3. Apptainer containers 101
4. A convenient apptainer containers mechanism
5. Apptainer containers for OpenFOAM
6. Concluding remarks

1› Introduction to Containers for HPCs

Write Code

1〉 Introduction to Containers for HPCs

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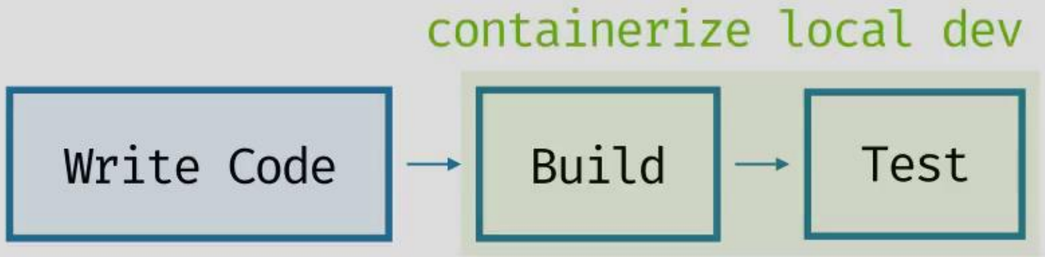

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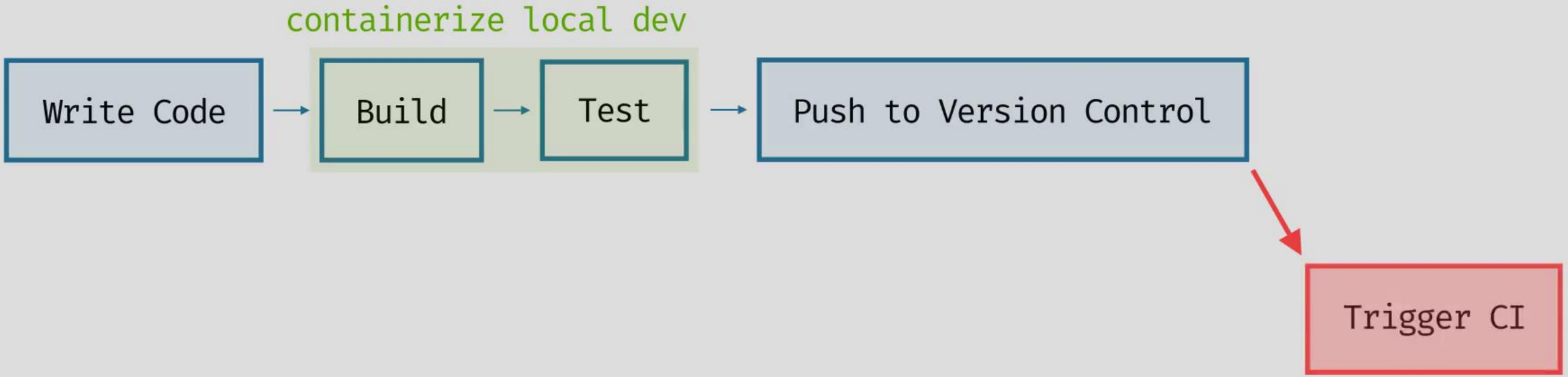

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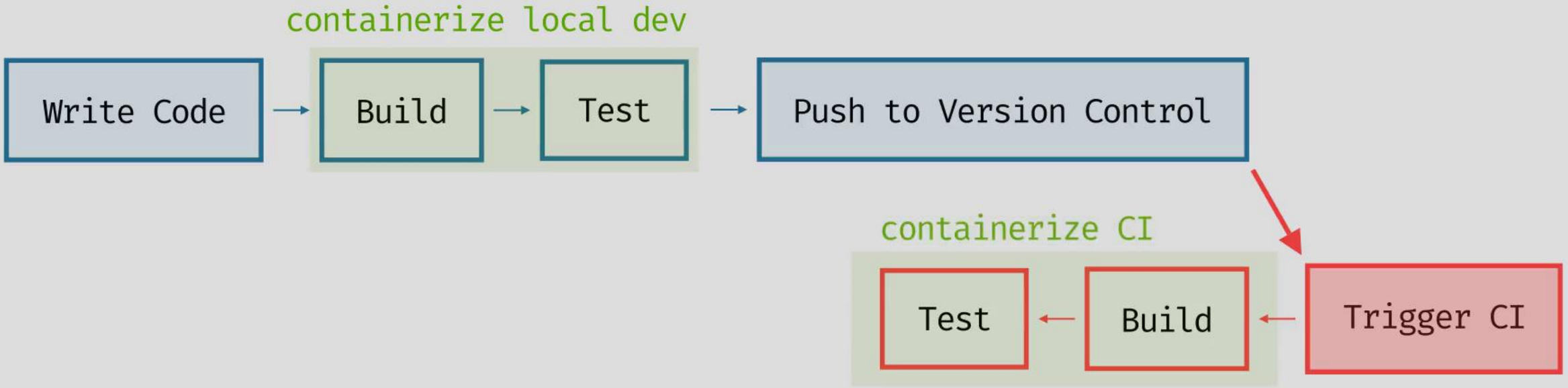

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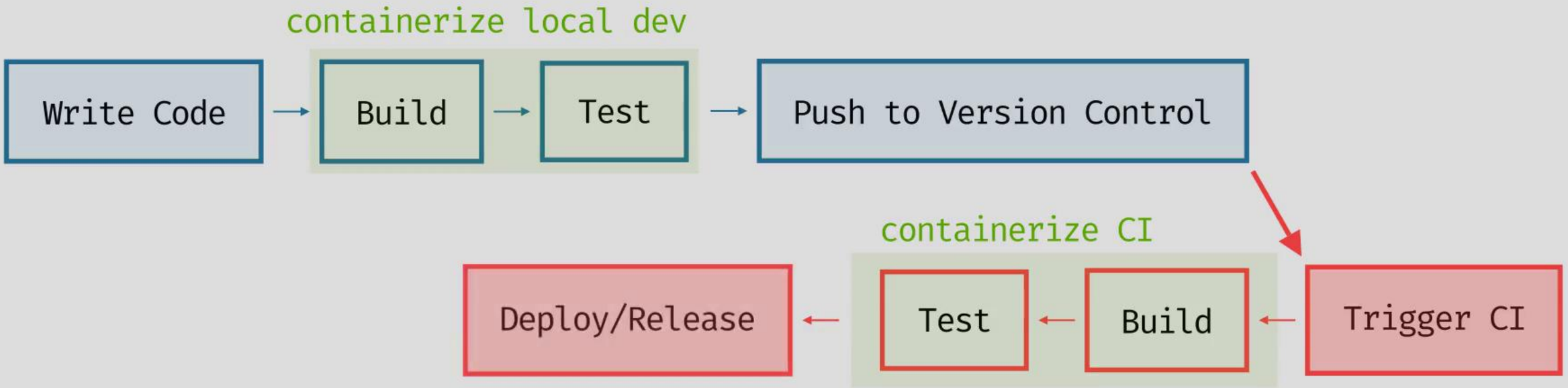

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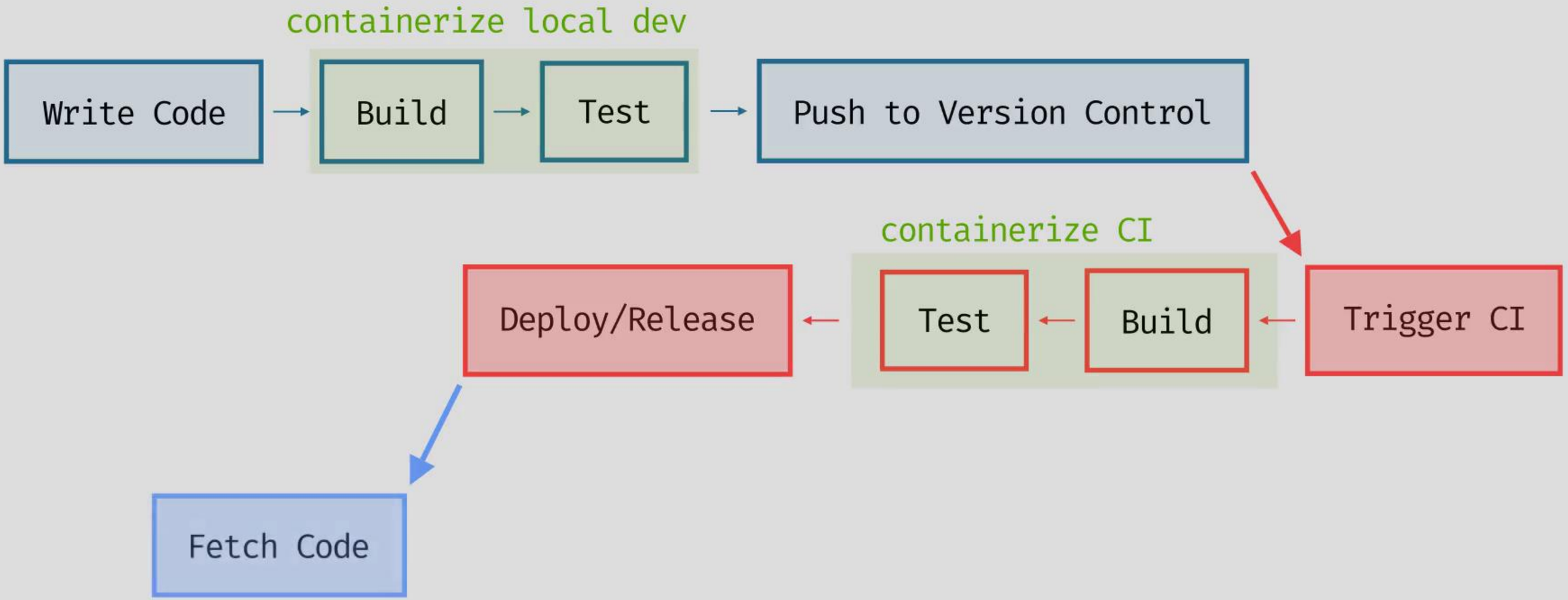

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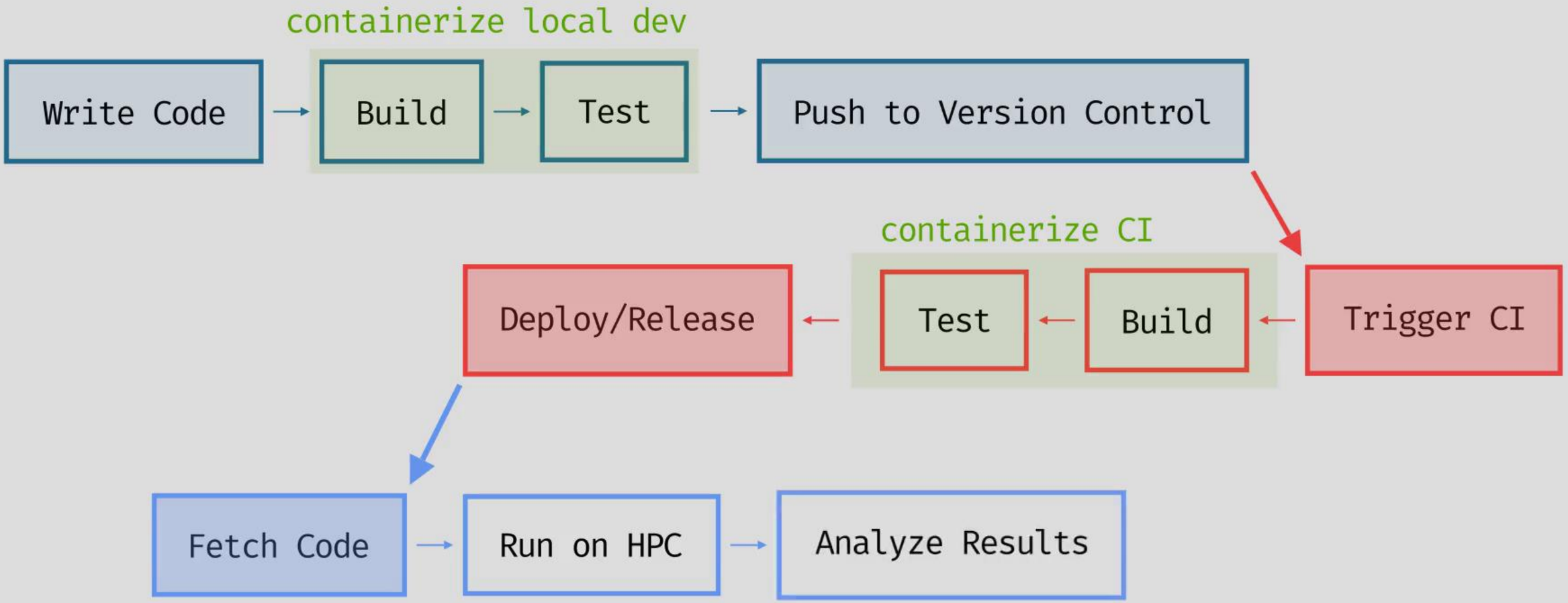

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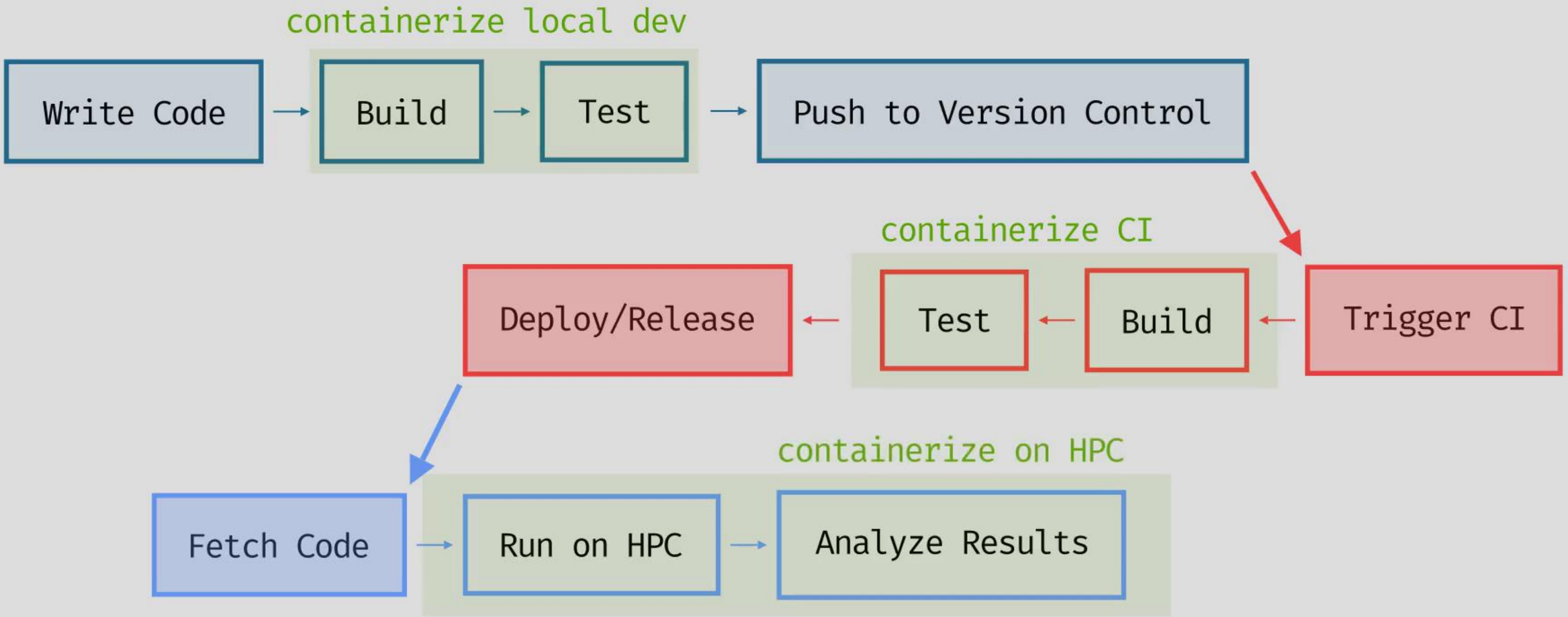

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Two common types for isolation

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Containers

Virtual machines

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1. Partial isolation from host
2. Uses host's Kernel
3. Controlled versionning of dependencies

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1. Full isolation from host
2. Dedicated resources
3. Provisionning overhead

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2. Dedicated resources
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Main Objective: cluster-agnostic sharing and reproducing of scientific workflows/data

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Two container usage aspects

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Two container usage aspects

Image creation and hosting

Container runs

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Two container usage aspects

Image creation and hosting

1. Build from definition files?
2. Can CI/CD build images?
3. Main purpose of the image?
4. Host images at public HUBs

Container runs

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Two container usage aspects

Image creation and hosting

1. Build from definition files?
2. Can CI/CD build images?
3. Main purpose of the image?
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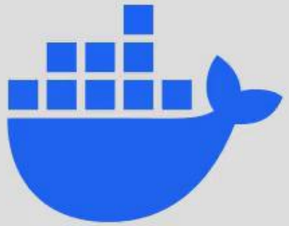
Container runs

1. MPI/Slurm compatibility?
2. Integration with HPC infrastructure
3. User convenience, even with minimal training
4. Security!!!

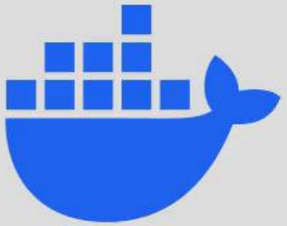
2❭ Cluster admins and container tech



Docker: most popular

2❭ Cluster admins and container tech

Podman: avoids Docker's daemon



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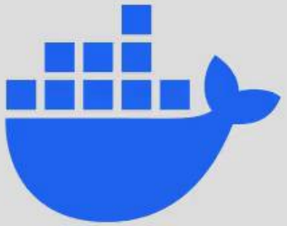

Docker: most popular

SARUS: HPC-focused

2❭ Cluster admins and container tech

Singularity: Single-Process-Execution

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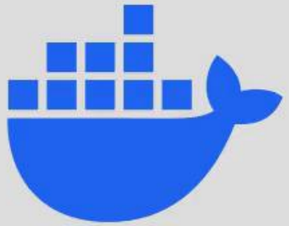

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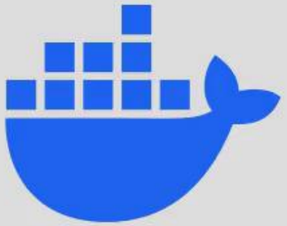

Docker: most popular

Apptainer: Modernized Singularity fork

SARUS: HPC-focused

3❭ Apptainer containers 101

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```
# definition file for a dummy image: test.def prodcing test.sif

Bootstrap: docker # or localimage
From: ubuntu:latest  # <- starting image









%runscript   # <- what to do when 'apptainer run image.sif'
    if [ $# -eq 0 ]; then /bin/bash; else /bin/bash -c "$@"; fi
```

3❭ Apptainer containers 101

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```
1   # definition file for a dummy image: test.def prodcing test.sif
2
3   Bootstrap: docker # or localimage
4   From: ubuntu:latest  # <- starting image
5
6   %post -c /bin/bash   # <- default is sh
7       echo "echo Sourced /bashrc" > /bashrc
8
9
10
11
12
13  %runscript   # <- what to do when 'apptainer run image.sif'
14      if [ $# -eq 0 ]; then /bin/bash; else /bin/bash -c "$@"; fi
```

3❭ Apptainer containers 101

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```
1  # definition file for a dummy image: test.def prodcing test.sif
2
3  Bootstrap: docker # or localimage
4  From: ubuntu:latest  # <- starting image
5
6  %post -c /bin/bash   # <- default is sh
7      echo "echo Sourced /bashrc" > /bashrc
8
9  %environment # <- set environment when run'ing/exec'ing
10     #!/bin/bash
11     source /bashrc
12
13 %runscript   # <- what to do when 'apptainer run image.sif'
14     if [ $# -eq 0 ]; then /bin/bash; else /bin/bash -c "$@"; fi
```

3❯ Apptainer containers 101

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```
apptainer build test.sif test.def # <- build test.sif image

apptainer run -C test.sif         # <- run in more isolated mode
apptainer run test.sif            # <- share env., PIDs... etc
apptainer run test.sif hostname   # <- run a command and exit

apptainer exec test.sif hostname  # <- skips %runscript

apptainer push test.sif oras://ghcr.io/USER/REPO:version
apptainer pull oras://ghcr.io/USER/REPO:version
```

4❭ A convenient apptainer containers mechanism

Automated container building based on YAML configs using Ansible

4❭ A convenient apptainer containers mechanism

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Automated container building based on YAML configs using Ansible

```yaml
containers:
  basic:
    opencfd-openfoam:
      os:
        distro: ubuntu
        version: 24.04
      mpi:
        implementation: openmpi
        version: 4.1.5
      framework:
        definition: com-openfoam
        version: 2312
        git_ref: default
```

4❭ A convenient apptainer containers mechanism

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      framework:
        definition: com-openfoam
        version: 2312
        git_ref: default
```

```yaml
projects:
  test:
    base_container: opencfd-openfoam
    definition: projects/test.def
    build_args:
      branch:
        - master
```

4❭ A convenient apptainer containers mechanism

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```
# Get dependency repo to a temp location
git clone https://github.com/FoamScience/openfoam-apptainer-packaging /tmp/tainers

# build (in this order):
#       containers/basic/ubuntu-24.04-openmpi-4.1.5.sif
#       containers/basic/opencfd-openfoam.sif
#       containers/projects/test-master.sif       <- your final container
# original dir is where your config.yaml is located
ansible-playbook /tmp/tainers build.yaml \
    --extra-vars "original_dir=$PWD" \
    --extra-vars "@config.yaml"
```

4❭ A convenient apptainer containers mechanism

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```
1   # definition files are now templated!
2
3   Bootstrap: localimage
4   From: {{ CONTAINERS_DIR }}/basic/{{ BASE_CONTAINER }}.sif
5
6   %post -c /bin/bash   # <- default is sh
7       echo "compiling {{ BRANCH }}"
8       # also, write meta data to /apps.json file
9
10  %environment #
11      #!/bin/bash
12      # unified sourcing of bashrcs and python envs here
13
14  %runscript   # <- always looks like this
15      if [ $# -eq 0 ]; then /bin/bash; else /bin/bash -c "$@"; fi
```

4❭ A convenient apptainer containers mechanism

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```
apptainer run containers/projects/test-master.sif info
```

4❭ A convenient apptainer containers mechanism

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```
apptainer run containers/projects/test-master.sif info
```

```
"openmpi": {
  "version": "4.1.5"
},
"openfoam": {
  "fork": "com-openfoam",
  "branch": "default",
  "commit": "default",
  "version": "2312"
},
```

```
"test": {
  "ompi_test": "/opt/OMPIFoam/ompiTest",
  "foam_test": "/opt/OMPIFoam/testOMPIFoam",
  "branch": "master"
}
```

5❭ Apptainer containers for OpenFOAM

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Scenario 1: OpenFOAM scalability study

5〉 Apptainer containers for OpenFOAM

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Scenario 1: OpenFOAM scalability study

1. Assume we have a configuration that builds a project in Opt/Debug modes
2. Want to add HPCToolkit to the Debug container
3. Upload the SIF file to multiple clusters and compare scalability

5〉 Apptainer containers for OpenFOAM

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Scenario 1: OpenFOAM scalability study

1. Assume we have a configuration that builds a project in Opt/Debug modes
2. Want to add HPCToolkit to the Debug container
3. Upload the SIF file to multiple clusters and compare scalability

1. The project's definition file is mostly a SHELL language
2. So, minimal maintenance overhead for the definition files
3. The YAML configuration file allows seamlessly stitching base containers!
4. Also, it allows loading your own base container definitions

5❭ Apptainer containers for OpenFOAM

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```
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####################################
```

5❭ Apptainer containers for OpenFOAM

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  basic:
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      os:
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        version: 24.04
      mpi:
        implementation: openmpi
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      framework:
        - definition: com-openfoam
          version: 2312
        - definition: hpctoolkit
          version: 2024.01.99-next
```

5❯ Apptainer containers for OpenFOAM

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containers:
  basic:
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      os:
        distro: ubuntu
        version: 24.04
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      framework:
        - definition: com-openfoam
          version: 2312
        - definition: hpctoolkit
          version: 2024.01.99-next
```

```yaml
projects:
  my_project:
    base_container: opencfd-openfoam
    definition: my_project.def
    build_args:
      mode:
        - Debug
```

5❭ Apptainer containers for OpenFOAM

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Scenario 2: Test things on a makeshift cluster

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Scenario 2: Test things on a makeshift cluster

1. Spawn Docker containers to act as "SLURM cluster" nodes
2. The nodes only need to have SLURM, Apptainer and some MPI installed
3. Build your container images locally
4. Upload them to the head node
5. Run the containers in MPI-hybrid mode

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5. Run the containers in MPI-hybrid mode

```
1  # from the head node, these should say same things
2  srun -N 3 hostname
3  srun -N 3 apptainer run my.sif hostname
4  # also valid if hostname were to support MPI
```

6〉 Concluding remarks

1. Single process execution is "the way to go" for HPC systems!
2. Automating containerization helps with dev productivity
3. Containers ease software/data sharing at frozen versions
4. Apptainer is still a bit under-supported on CI/CD systems

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For all asssociated materials, and the slides:

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For all asssociated materials, and the slides:

1. https://github.com/FoamScience/lichtenberg-training-apptainers-presentation
2. https://foamscience.github.io/lichtenberg-training-apptainers-presentation

THANK YOU for your attention!