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Software Quality Assurance for High Performance Computing Containers utilizing MVAPICH2 and the MOOSE framework

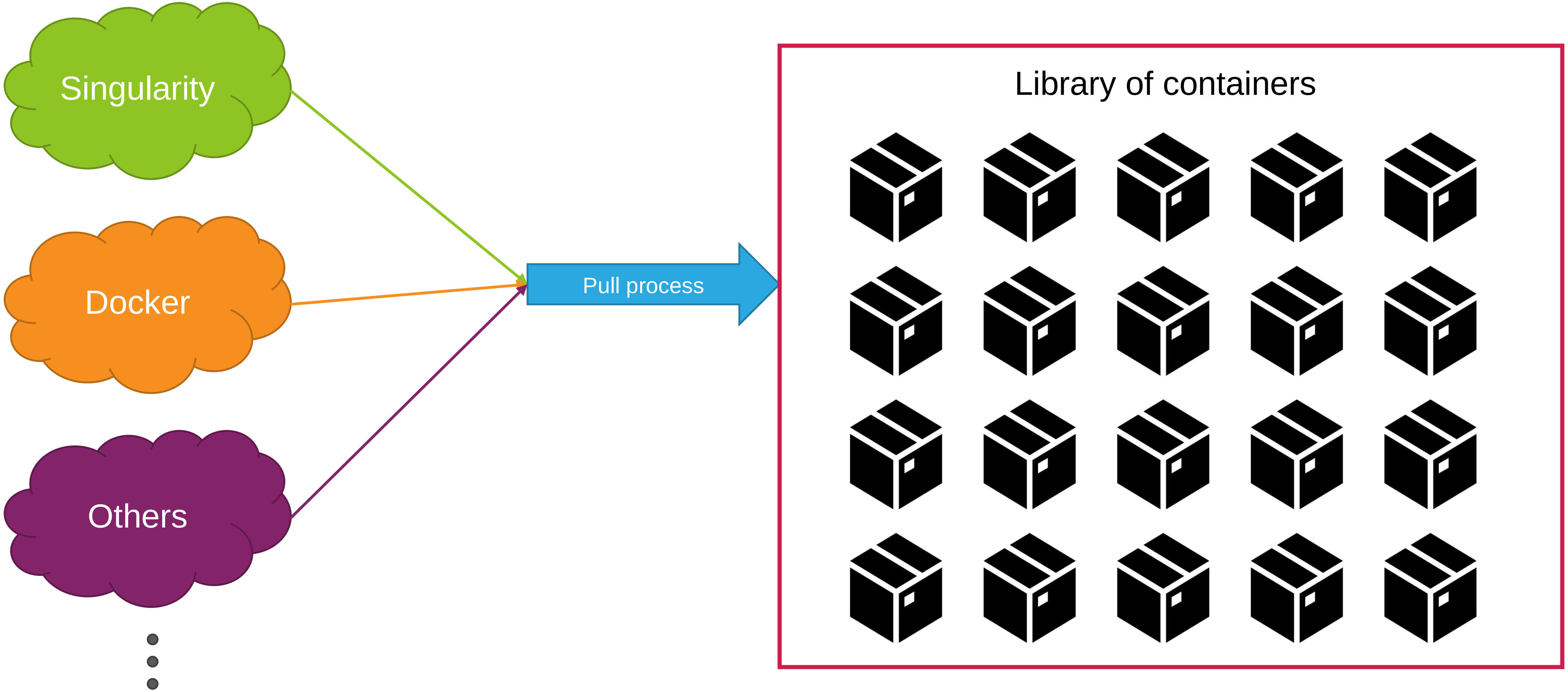
MUG 2023

INL/CON-23-74293

Why containers?

- Verification and Validation: Is my code running correctly still? Is it passing all unit tests and giving the same results as my last few papers?
- Reproducibility: Can I run my same application 10 years later? Can I rebuild my container 10 years later?
- Portability across multiple supercomputer architectures: Can I run the same container on multiple supercomputers with different networks and drivers *without rebuilding and without sacrificing performance*?
- Simplification: one environment, customized packages (independence from system administrators); make it easier on the user: Can I work without needing intervention from the system administrator?
- Security (insulation against package versioning issues): Does a security update on a supercomputer break my code?

Containers – Creation



Singularity

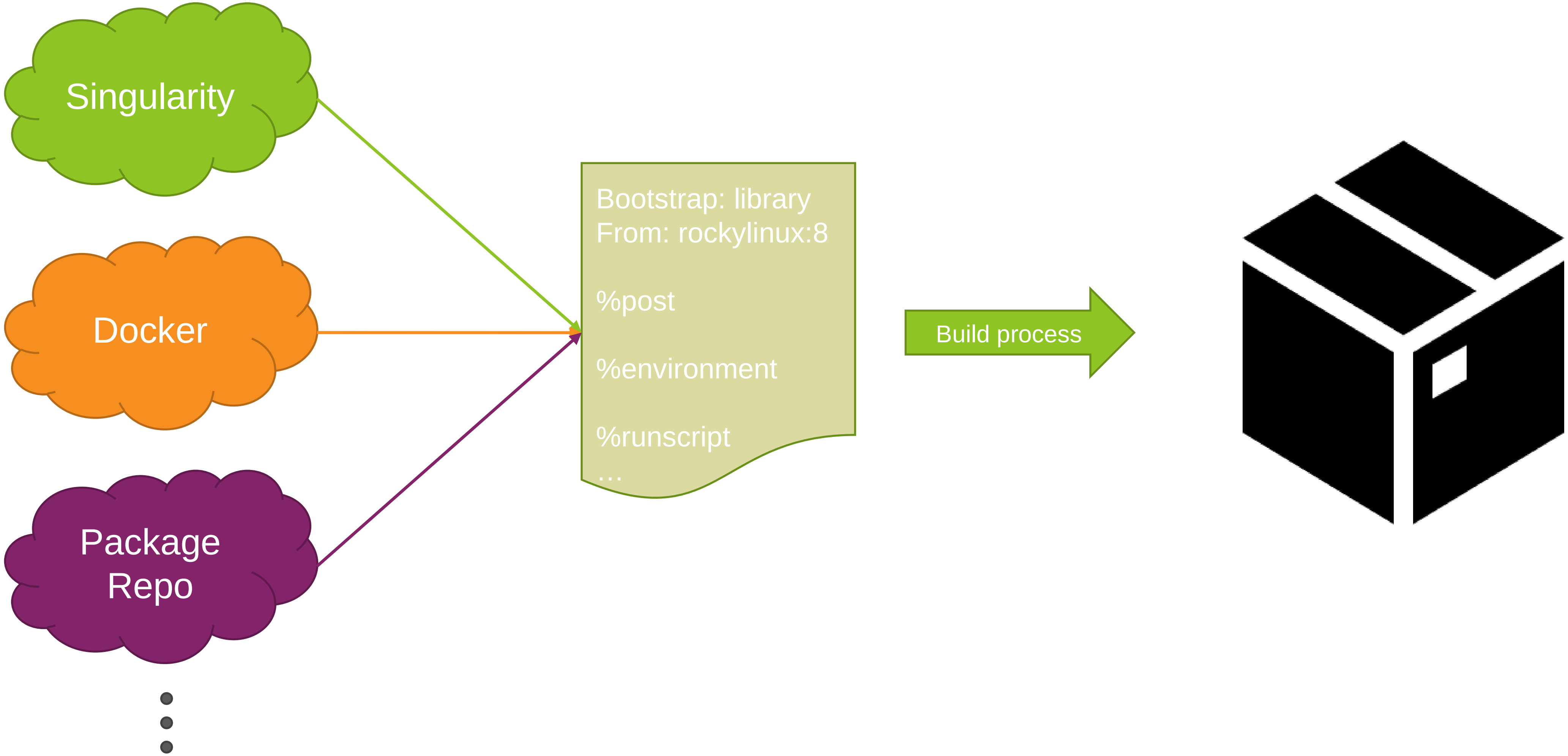
Docker

Others

Pull process

Library of containers

Create a container with def file



Singularity

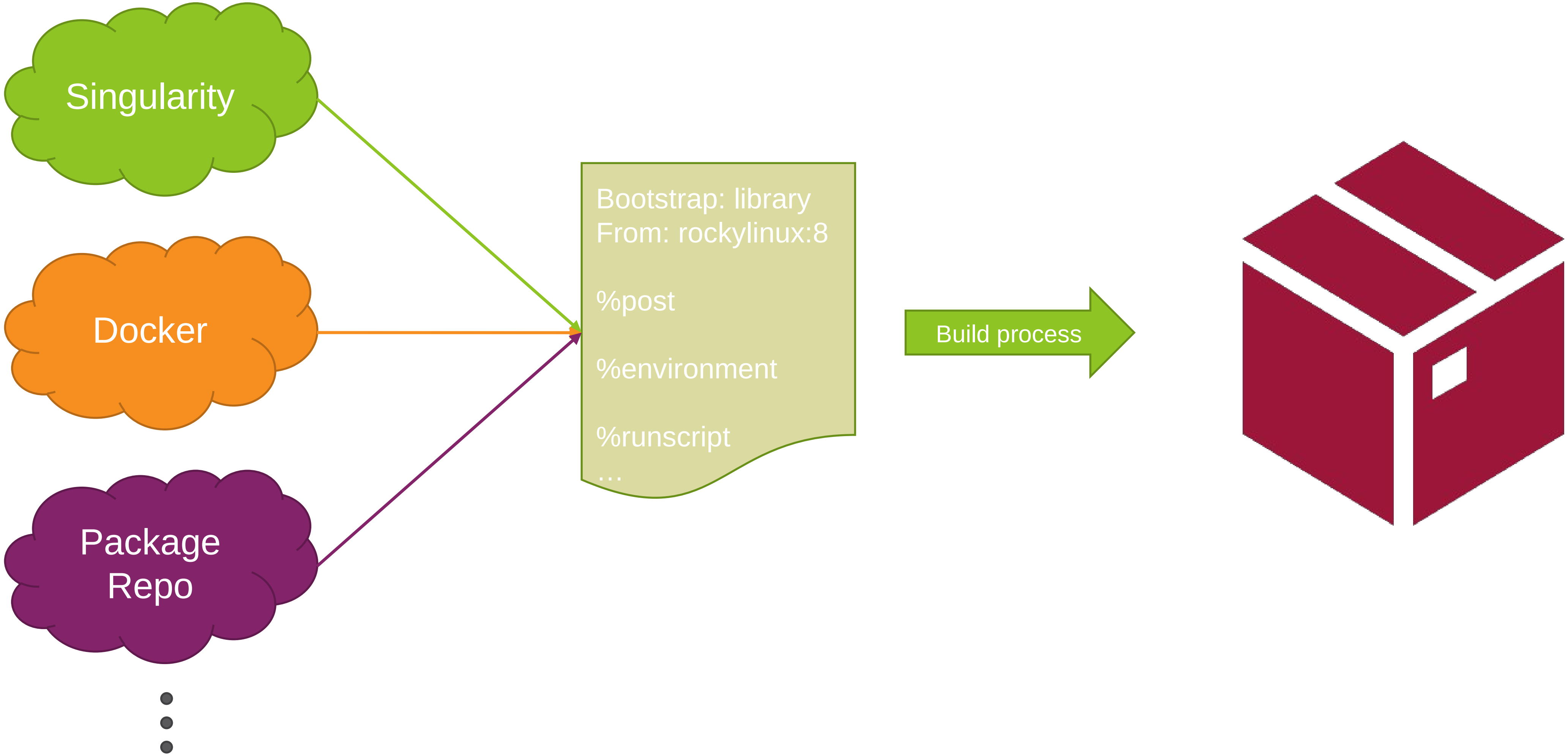
Docker

Package Repo

```
Bootstrap: library
From: rockylinux:8

%post

%environment

%runscript
…
```

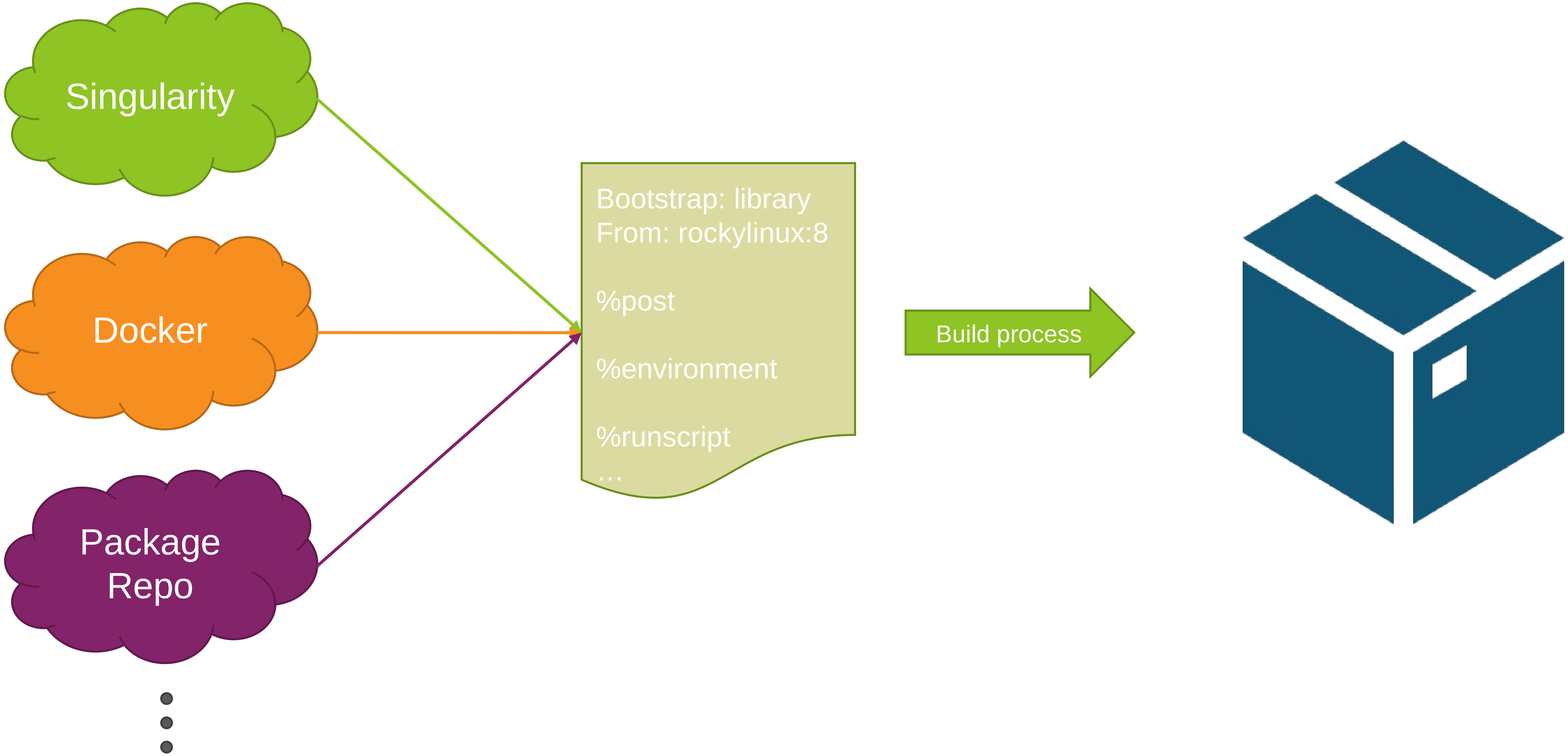
Build process

Create a container – Reproduceable?



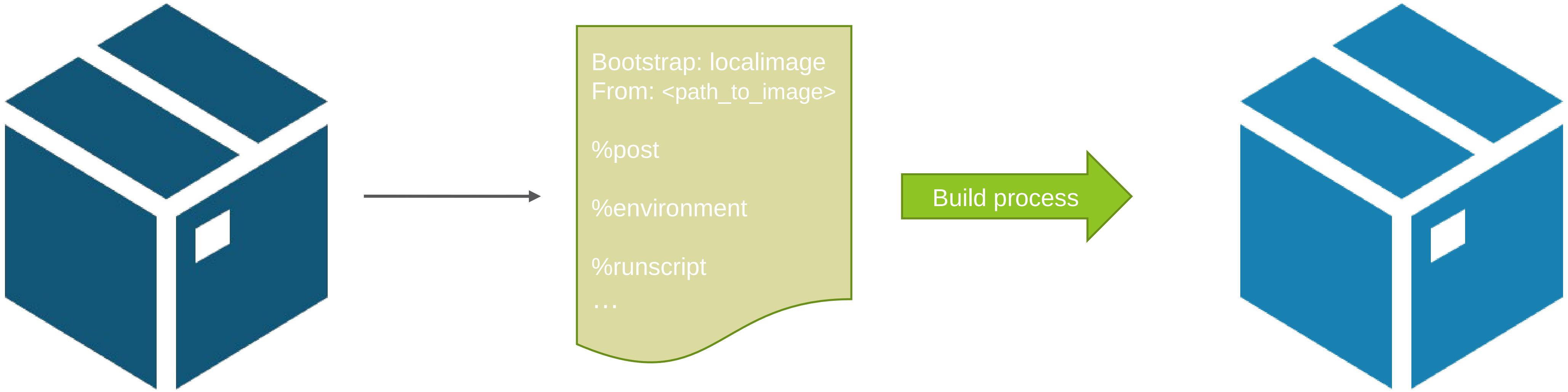
```
Bootstrap: library
From: rockylinux:8

%post

%environment

%runscript
…
```

Create a container – Reproduceable?
Layer system



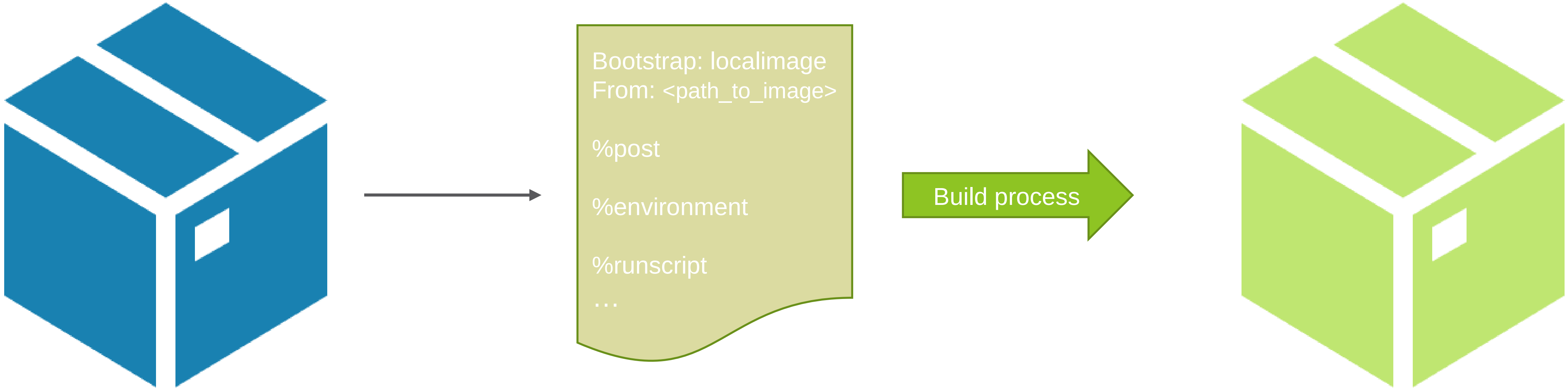
```
Bootstrap: library
From: rockylinux:8

%post

%environment

%runscript
…
```

Create a container – Reproduceable?
Layer system



```
Bootstrap: localimage
From: <path_to_image>

%post

%environment

%runscript
…
```

Create a container – Reproduceable?
Layer system



```
Bootstrap: localimage
From: <path_to_image>

%post

%environment

%runscript
…
```

Build process

Containers with MPI and IB – Two Approaches

- Hybrid
  - System MPI
  - Container MPI
  - System IB
  - Container IB

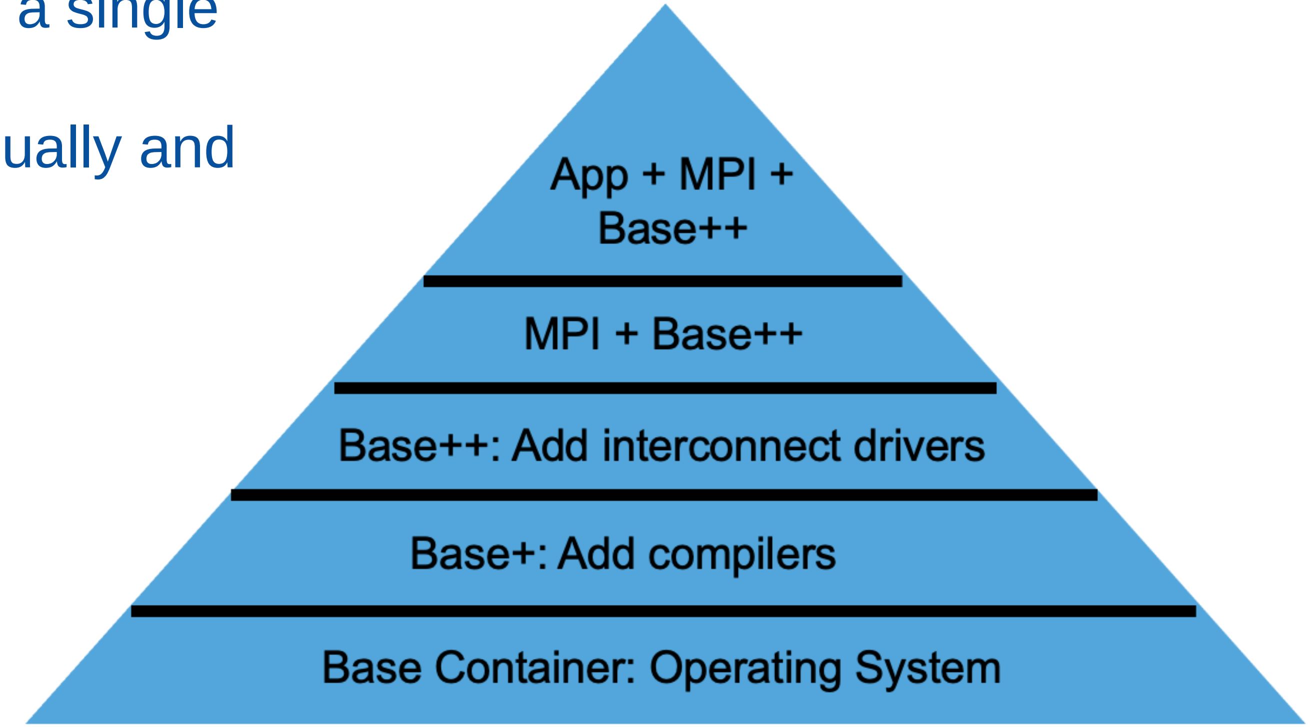
- Bind
  - System MPI
  - System IB

NOTE:

This requires the Host OS and Container OS to be compatible

Container Strategy

- There are three key components to the strategy:
  - HPC application containers built via layers
  - Key components are grouped into a single layer
  - Each layer can be updated individually and reproducibly via local mirrors



App + MPI + Base++

MPI + Base++

Base++: Add interconnect drivers

Base+: Add compilers

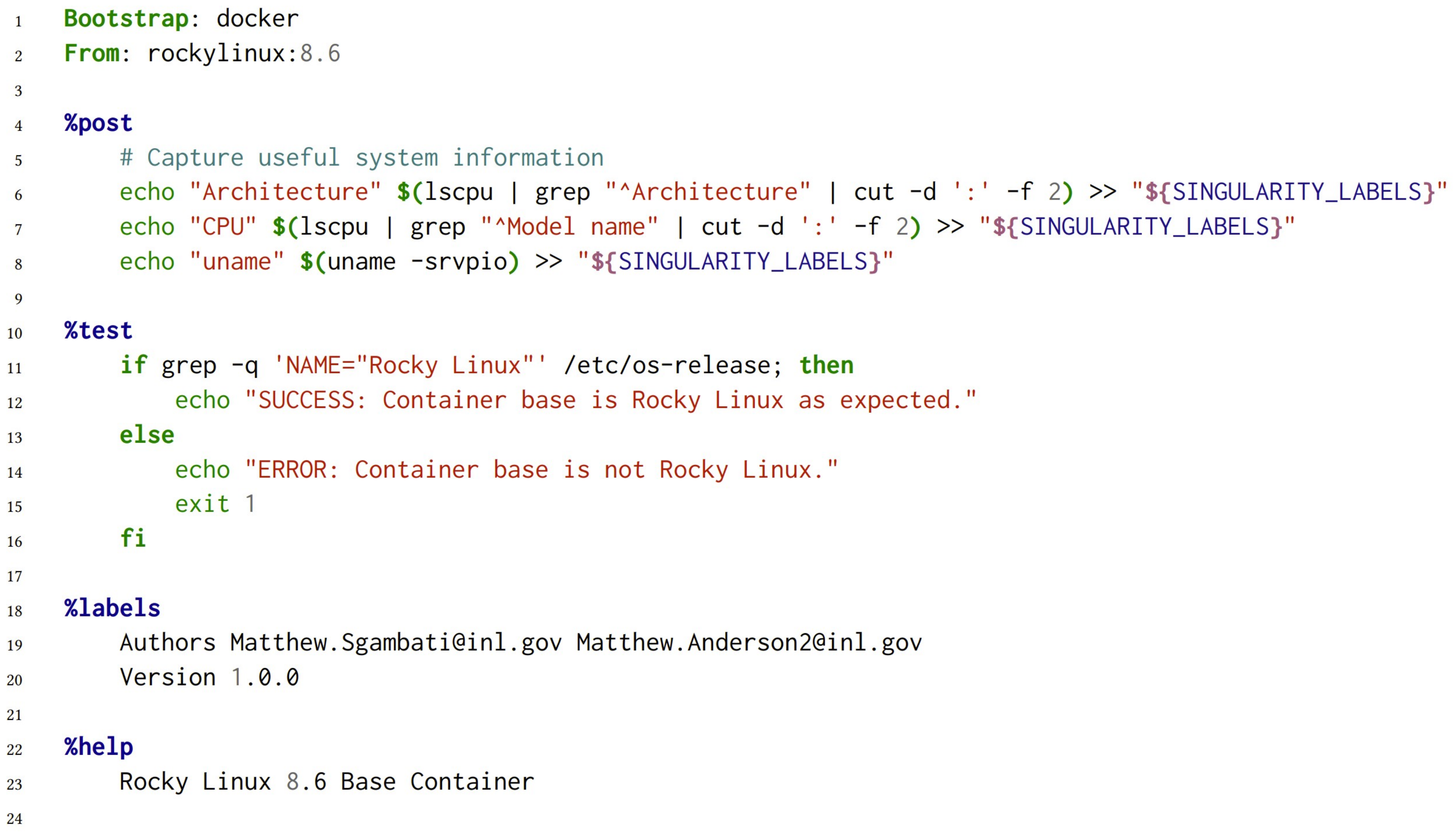
Base Container: Operating System

Container Strategy – Assumptions

- Host systems will use a long-term support (LTS) version of drivers and/or software stacks when possible
- Host system administrators will install an ABI-compatible version of MPI if one does not exist on the target system

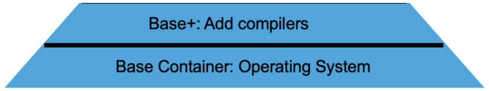
Base Container Definition File

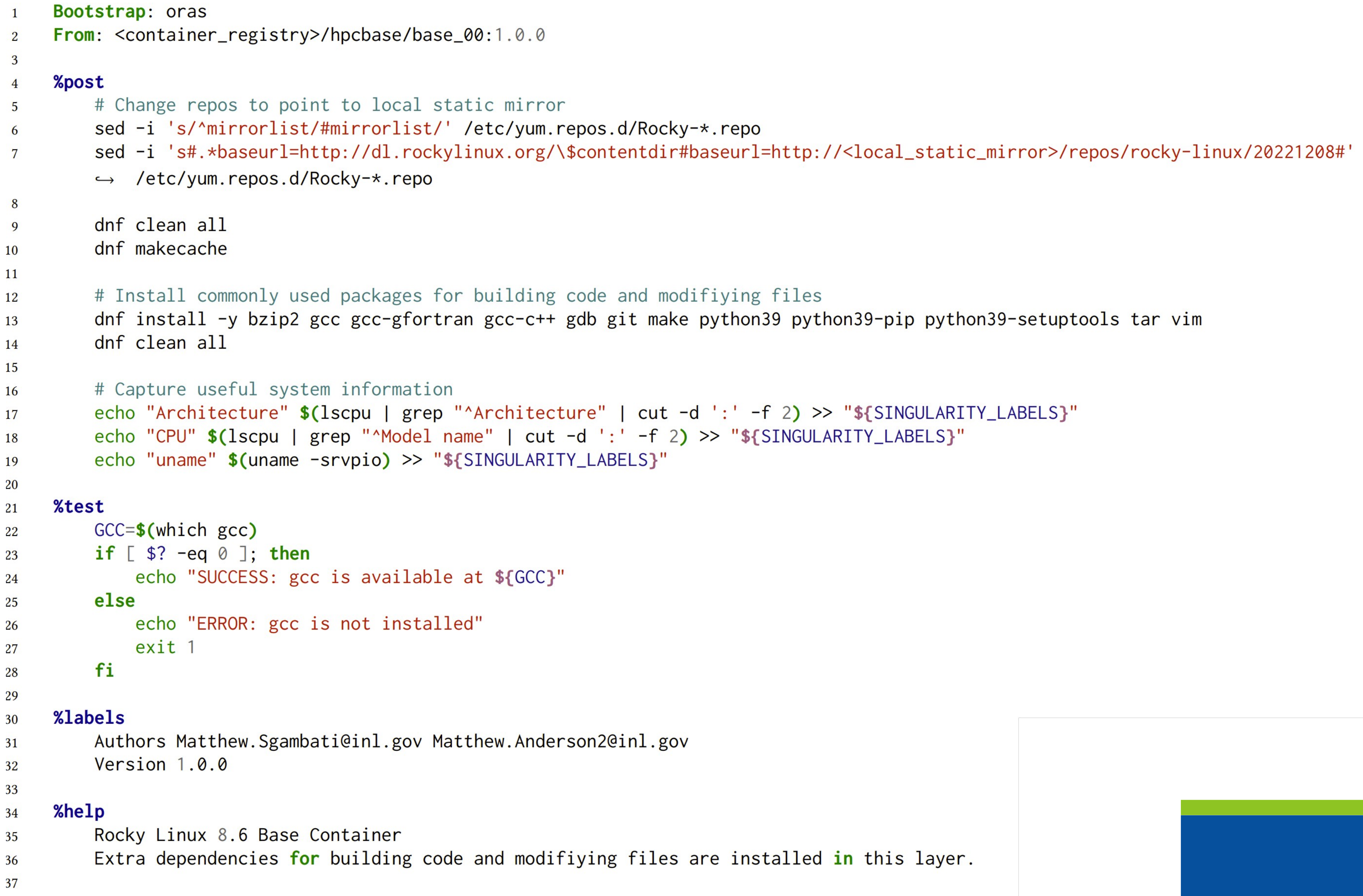
Base Container: Operating System



```
Bootstrap: docker
From: rockylinux:8.6

%post
    # Capture useful system information
    echo "Architecture" $(lscpu | grep "^Architecture" | cut -d ':' -f 2) >> "${SINGULARITY_LABELS}"
    echo "CPU" $(lscpu | grep "^Model name" | cut -d ':' -f 2) >> "${SINGULARITY_LABELS}"
    echo "uname" $(uname -srvpio) >> "${SINGULARITY_LABELS}"

%test
    if grep -q 'NAME="Rocky Linux"' /etc/os-release; then
        echo "SUCCESS: Container base is Rocky Linux as expected."
    else
        echo "ERROR: Container base is not Rocky Linux."
        exit 1
    fi

%labels
    Authors Matthew.Sgambati@inl.gov Matthew.Anderson2@inl.gov
    Version 1.0.0

%help
    Rocky Linux 8.6 Base Container

```

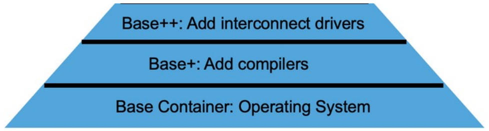
Base+ Container Definition File

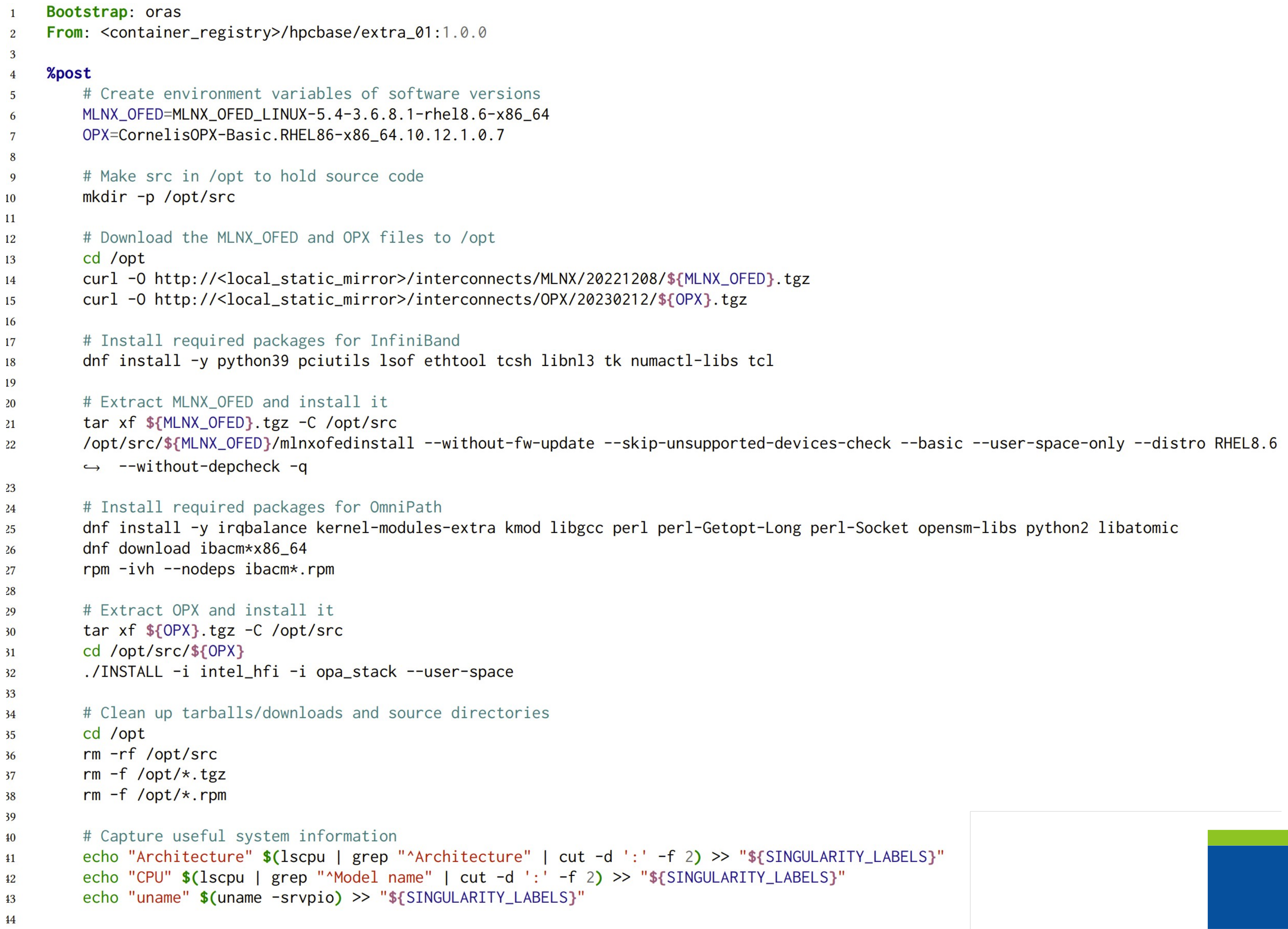




```
Bootstrap: oras
From: <container_registry>/hpcbase/base_00:1.0.0

%post
    # Change repos to point to local static mirror
    sed -i 's/^mirrorlist/#mirrorlist/' /etc/yum.repos.d/Rocky-*.repo
    sed -i 's#.*baseurl=http://dl.rockylinux.org/\$contentdir#baseurl=http://<local_static_mirror>/repos/rocky-linux/20221208#' /etc/yum.repos.d/Rocky-*.repo

    dnf clean all
    dnf makecache

    # Install commonly used packages for building code and modifiying files
    dnf install -y bzip2 gcc gcc-gfortran gcc-c++ gdb git make python39 python39-pip python39-setuptools tar vim
    dnf clean all

    # Capture useful system information
    echo "Architecture" $(lscpu | grep "^Architecture" | cut -d ':' -f 2) >> "${SINGULARITY_LABELS}"
    echo "CPU" $(lscpu | grep "^Model name" | cut -d ':' -f 2) >> "${SINGULARITY_LABELS}"
    echo "uname" $(uname -srvpio) >> "${SINGULARITY_LABELS}"

%test
    GCC=$(which gcc)
    if [ $? -eq 0 ]; then
        echo "SUCCESS: gcc is available at ${GCC}"
    else
        echo "ERROR: gcc is not installed"
        exit 1
    fi

%labels
    Authors Matthew.Sgambati@inl.gov Matthew.Anderson2@inl.gov
    Version 1.0.0

%help
    Rocky Linux 8.6 Base Container
    Extra dependencies for building code and modifiying files are installed in this layer.
```

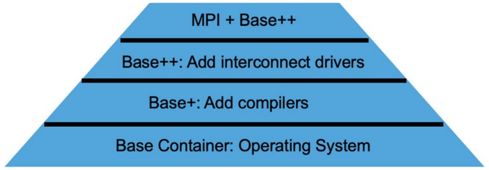
Base++ Container Definition File

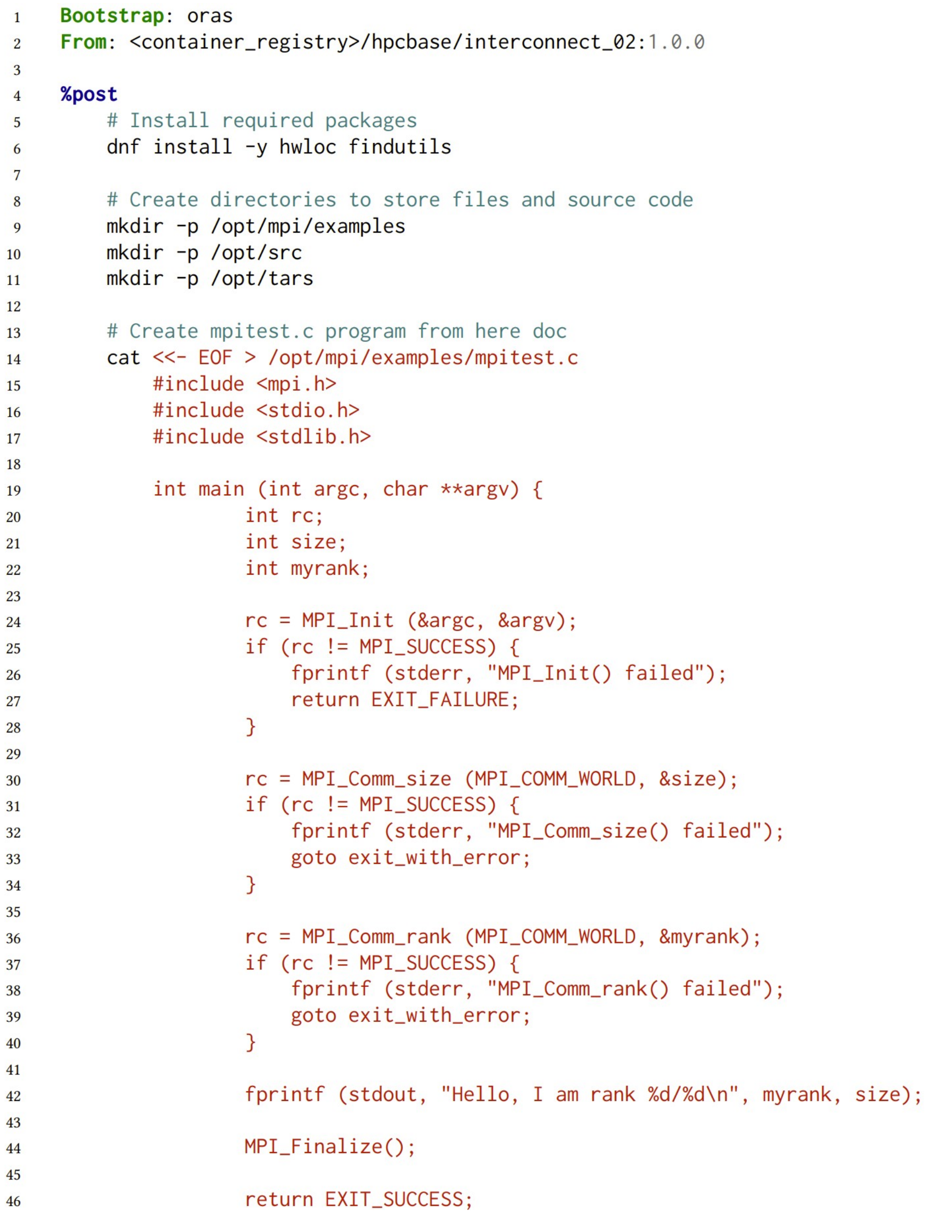

Base++: Add interconnect drivers
Base+: Add compilers
Base Container: Operating System



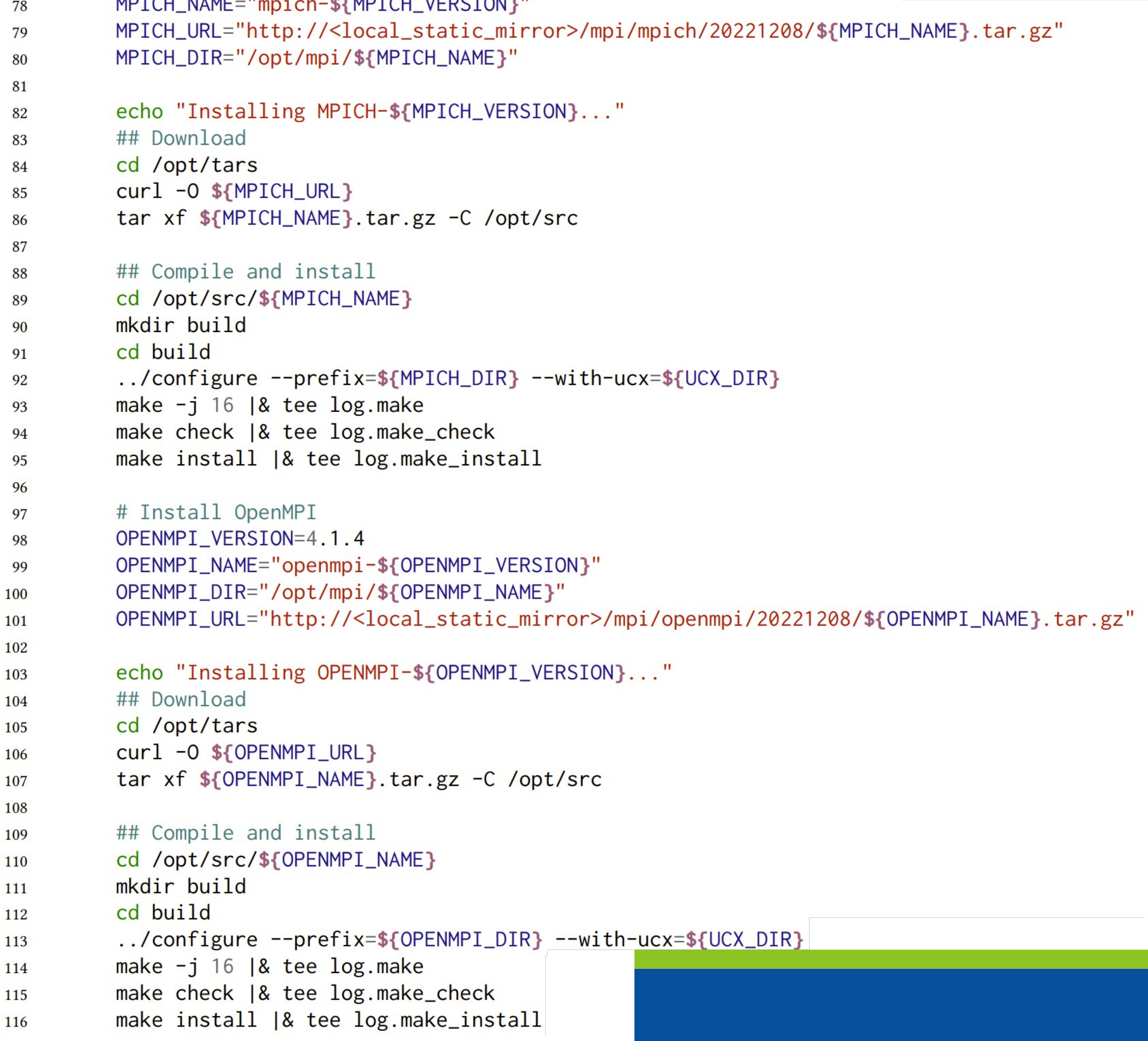
```
Bootstrap: oras
From: <container_registry>/hpcbase/extra_01:1.0.0

%post
    # Create environment variables of software versions
    MLNX_OFED=MLNX_OFED_LINUX-5.4-3.6.8.1-rhel8.6-x86_64
    OPX=CornelisOPX-Basic.RHEL86-x86_64.10.12.1.0.7

    # Make src in /opt to hold source code
    mkdir -p /opt/src

    # Download the MLNX_OFED and OPX files to /opt
    cd /opt
    curl -O http://<local_static_mirror>/interconnects/MLNX/20221208/${MLNX_OFED}.tgz
    curl -O http://<local_static_mirror>/interconnects/OPX/20230212/${OPX}.tgz

    # Install required packages for InfiniBand
    dnf install -y python39 pciutils lsof ethtool tcsh libnl3 tk numactl-libs tcl

    # Extract MLNX_OFED and install it
    tar xf ${MLNX_OFED}.tgz -C /opt/src
    /opt/src/${MLNX_OFED}/mlnxofedinstall --without-fw-update --skip-unsupported-devices-check --basic --user-space-only --distro RHEL8.6
    ↪  --without-depcheck -q

    # Install required packages for OmniPath
    dnf install -y irqbalance kernel-modules-extra kmod libgcc perl perl-Getopt-Long perl-Socket opensm-libs python2 libatomic
    dnf download ibacm*x86_64
    rpm -ivh --nodeps ibacm*.rpm

    # Extract OPX and install it
    tar xf ${OPX}.tgz -C /opt/src
    cd /opt/src/${OPX}
    ./INSTALL -i intel_hfi -i opa_stack --user-space

    # Clean up tarballs/downloads and source directories
    cd /opt
    rm -rf /opt/src
    rm -f /opt/*.tgz
    rm -f /opt/*.rpm

    # Capture useful system information
    echo "Architecture" $(lscpu | grep "^Architecture" | cut -d ':' -f 2) >> "${SINGULARITY_LABELS}"
    echo "CPU" $(lscpu | grep "^Model name" | cut -d ':' -f 2) >> "${SINGULARITY_LABELS}"
    echo "uname" $(uname -srvpio) >> "${SINGULARITY_LABELS}"

```

MPI + Base++ Container Definition File


MPI + Base++
Base++: Add interconnect drivers
Base+: Add compilers
Base Container: Operating System

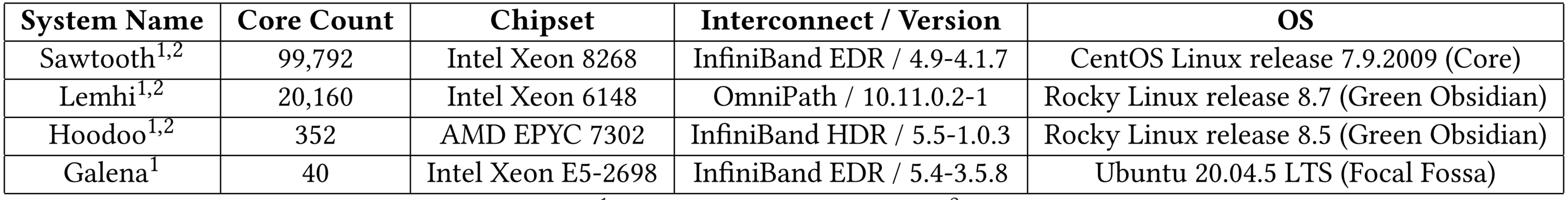


```
Bootstrap: oras
From: <container_registry>/hpcbase/interconnect_02:1.0.0

%post
    # Install required packages
    dnf install -y hwloc findutils

    # Create directories to store files and source code
    mkdir -p /opt/mpi/examples
    mkdir -p /opt/src
    mkdir -p /opt/tars

    # Create mpitest.c program from here doc
    cat <<- EOF > /opt/mpi/examples/mpitest.c
        #include <mpi.h>
        #include <stdio.h>
        #include <stdlib.h>

        int main (int argc, char **argv) {
                int rc;
                int size;
                int myrank;

                rc = MPI_Init (&argc, &argv);
                if (rc != MPI_SUCCESS) {
                    fprintf (stderr, "MPI_Init() failed");
                    return EXIT_FAILURE;
                }

                rc = MPI_Comm_size (MPI_COMM_WORLD, &size);
                if (rc != MPI_SUCCESS) {
                    fprintf (stderr, "MPI_Comm_size() failed");
                    goto exit_with_error;
                }

                rc = MPI_Comm_rank (MPI_COMM_WORLD, &myrank);
                if (rc != MPI_SUCCESS) {
                    fprintf (stderr, "MPI_Comm_rank() failed");
                    goto exit_with_error;
                }

                fprintf (stdout, "Hello, I am rank %d/%d\n", myrank, size);

                MPI_Finalize();

                return EXIT_SUCCESS;
```



```
    # Install MPICH
    MPICH_VERSION=3.4.3
    MPICH_NAME="mpich-${MPICH_VERSION}"
    MPICH_URL="http://<local_static_mirror>/mpi/mpich/20221208/${MPICH_NAME}.tar.gz"
    MPICH_DIR="/opt/mpi/${MPICH_NAME}"

    echo "Installing MPICH-${MPICH_VERSION}..."
    ## Download
    cd /opt/tars
    curl -O ${MPICH_URL}
    tar xf ${MPICH_NAME}.tar.gz -C /opt/src

    ## Compile and install
    cd /opt/src/${MPICH_NAME}
    mkdir build
    cd build
    ../configure --prefix=${MPICH_DIR} --with-ucx=${UCX_DIR}
    make -j 16 |& tee log.make
    make check |& tee log.make_check
    make install |& tee log.make_install

    # Install OpenMPI
    OPENMPI_VERSION=4.1.4
    OPENMPI_NAME="openmpi-${OPENMPI_VERSION}"
    OPENMPI_DIR="/opt/mpi/${OPENMPI_NAME}"
    OPENMPI_URL="http://<local_static_mirror>/mpi/openmpi/20221208/${OPENMPI_NAME}.tar.gz"

    echo "Installing OPENMPI-${OPENMPI_VERSION}..."
    ## Download
    cd /opt/tars
    curl -O ${OPENMPI_URL}
    tar xf ${OPENMPI_NAME}.tar.gz -C /opt/src

    ## Compile and install
    cd /opt/src/${OPENMPI_NAME}
    mkdir build
    cd build
    ../configure --prefix=${OPENMPI_DIR} --with-ucx=${UCX_DIR}
    make -j 16 |& tee log.make
    make check |& tee log.make_check
    make install |& tee log.make_install
```

Container Systems for Testing



System Name	Core Count	Chipset	Interconnect / Version	OS
Sawtooth[1,2]	99,792	Intel Xeon 8268	InfiniBand EDR / 4.9-4.1.7	CentOS Linux release 7.9.2009 (Core)
Lemhi[1,2]	20,160	Intel Xeon 6148	OmniPath / 10.11.0.2-1	Rocky Linux release 8.7 (Green Obsidian)
Hoodoo[1,2]	352	AMD EPYC 7302	InfiniBand HDR / 5.5-1.0.3	Rocky Linux release 8.5 (Green Obsidian)
Galena[1]	40	Intel Xeon E5-2698	InfiniBand EDR / 5.4-3.5.8	Ubuntu 20.04.5 LTS (Focal Fossa)

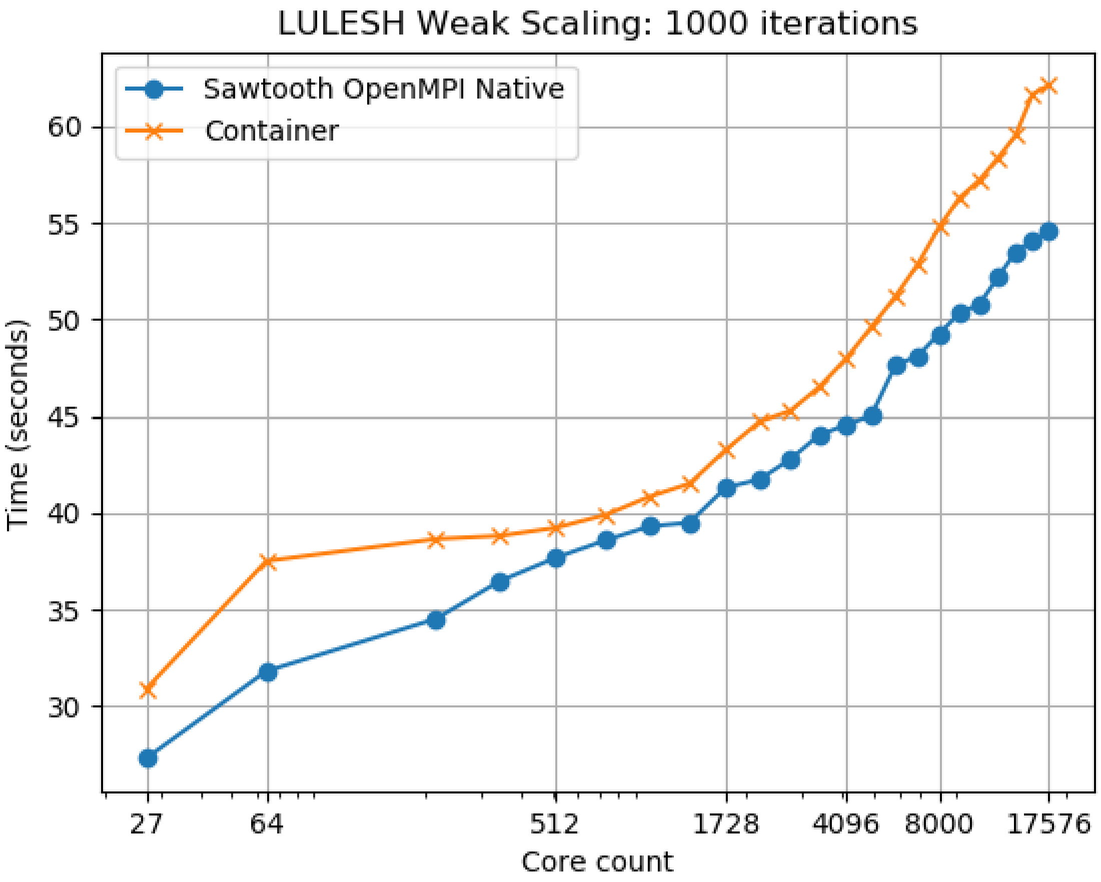
Sawtooth

Lemhi

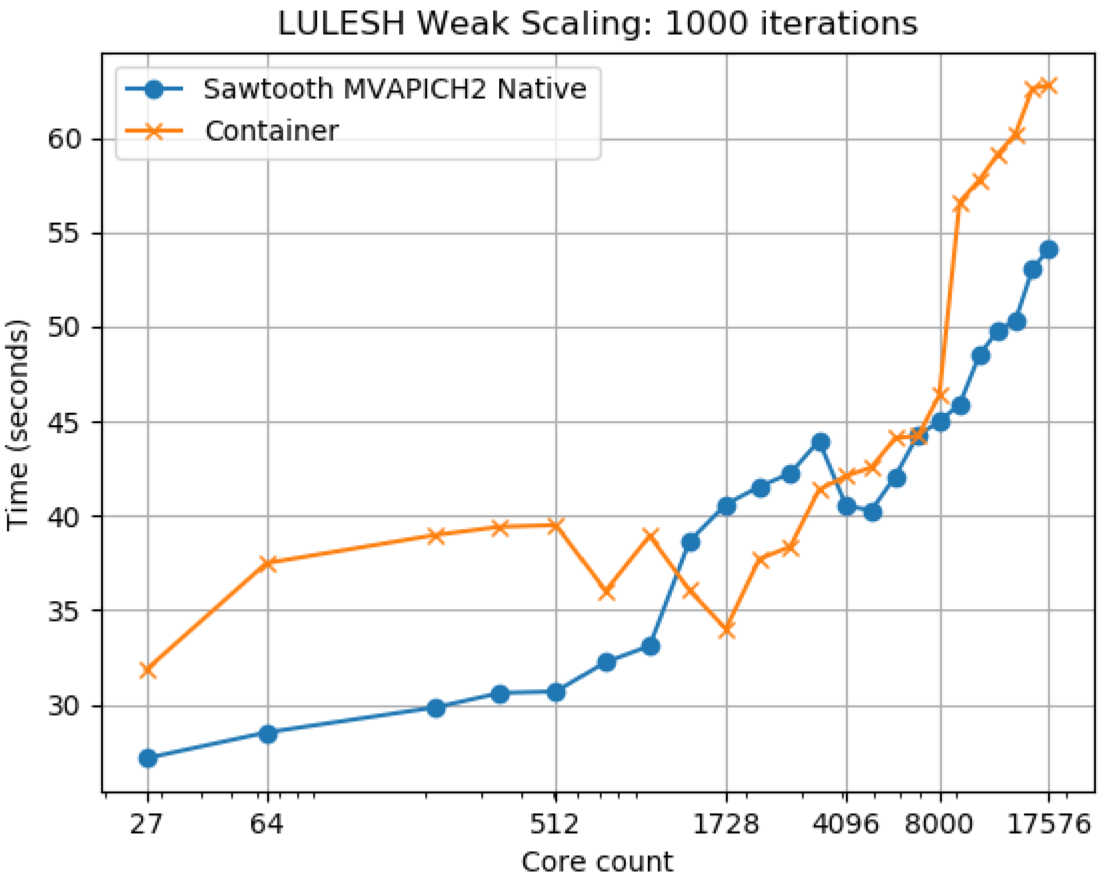
Hoodoo

Galena

LULESH – Sawtooth

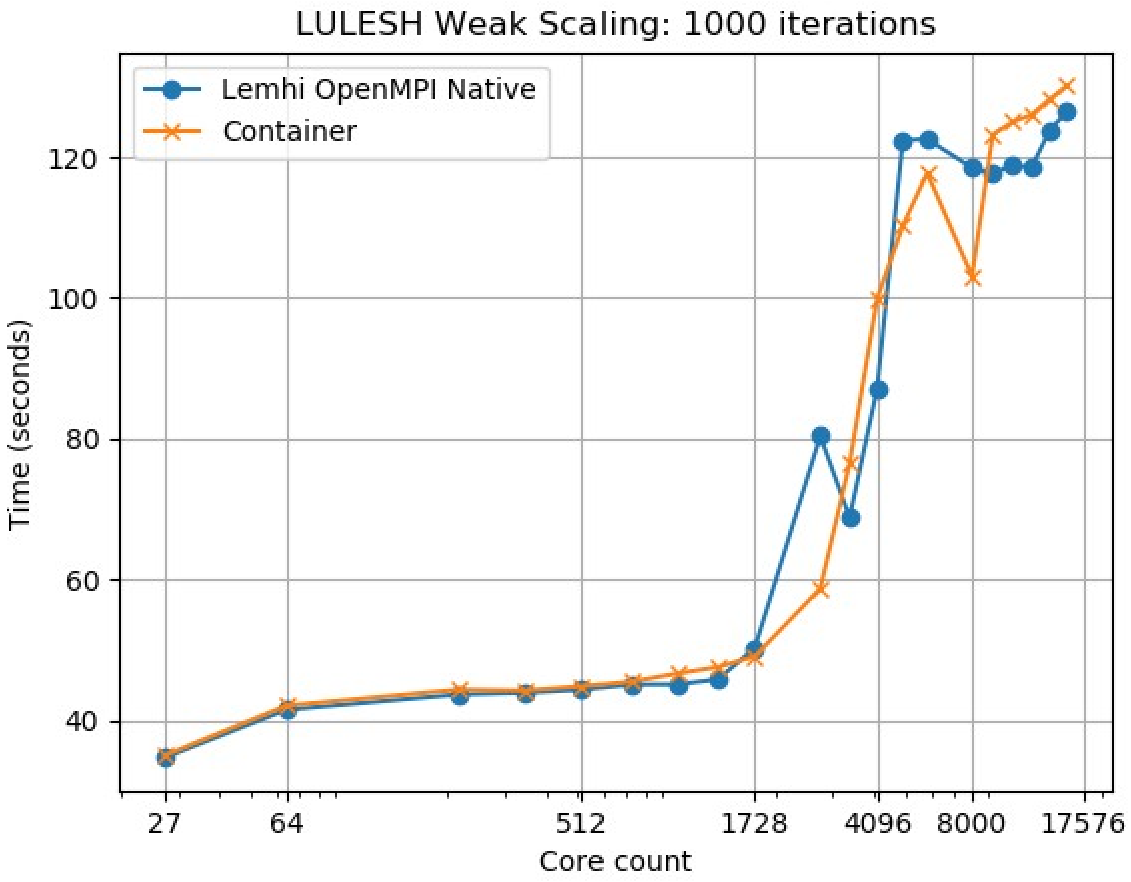


OpenMPI 4.1.4

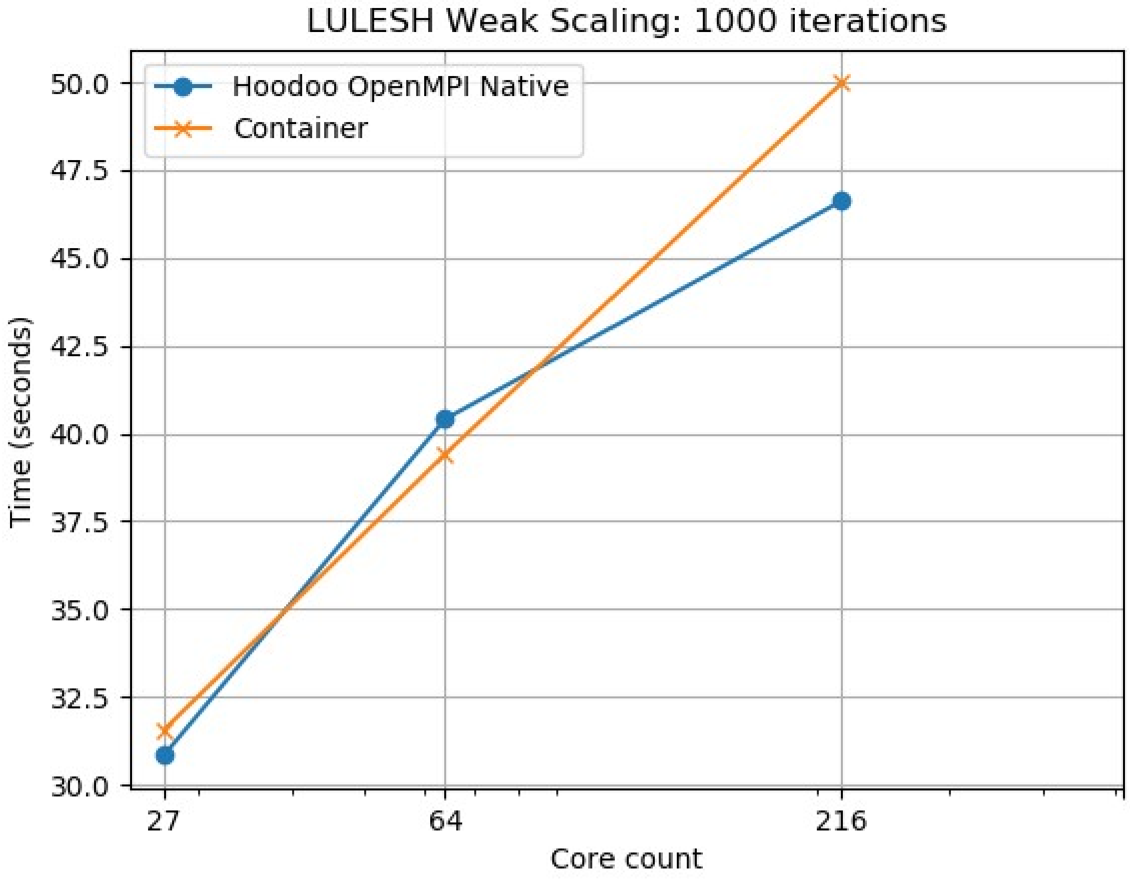


MVAPICH2 2.3.5

LULESH – Lemhi and Hoodoo

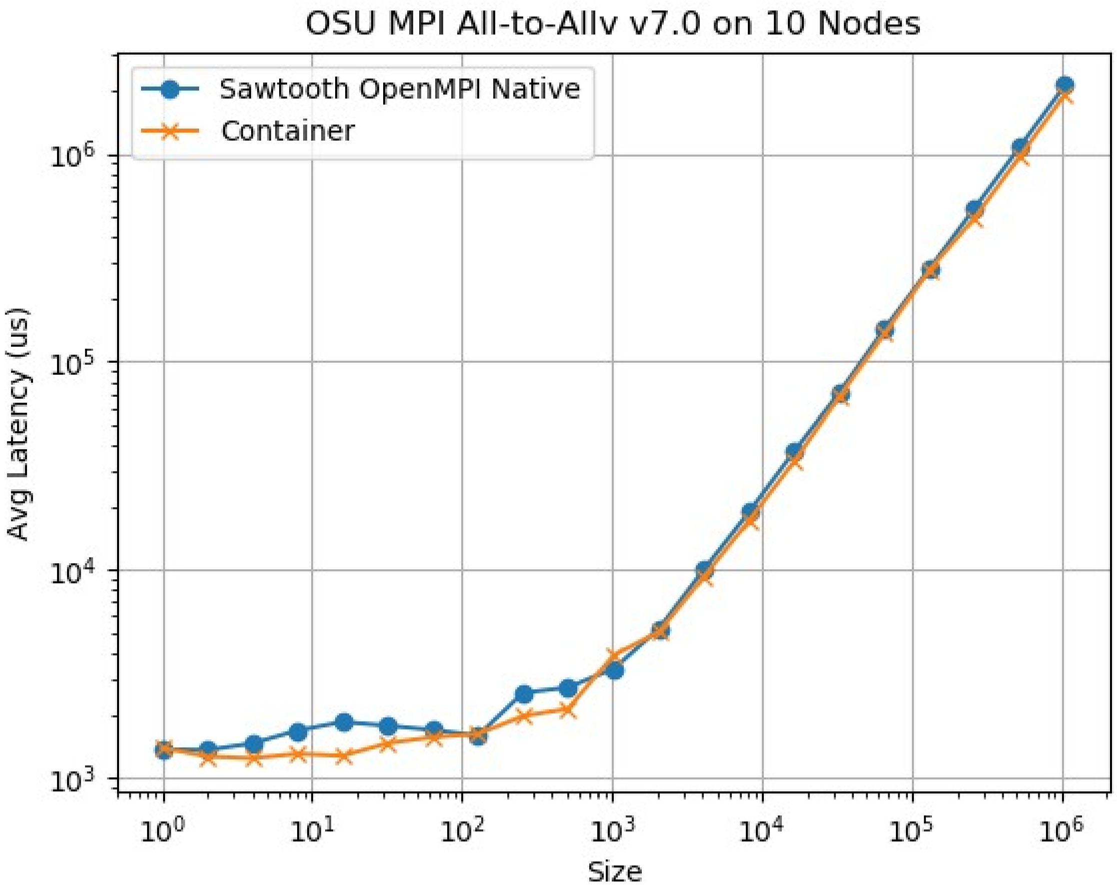


Lemhi
OpenMPI 4.1.1

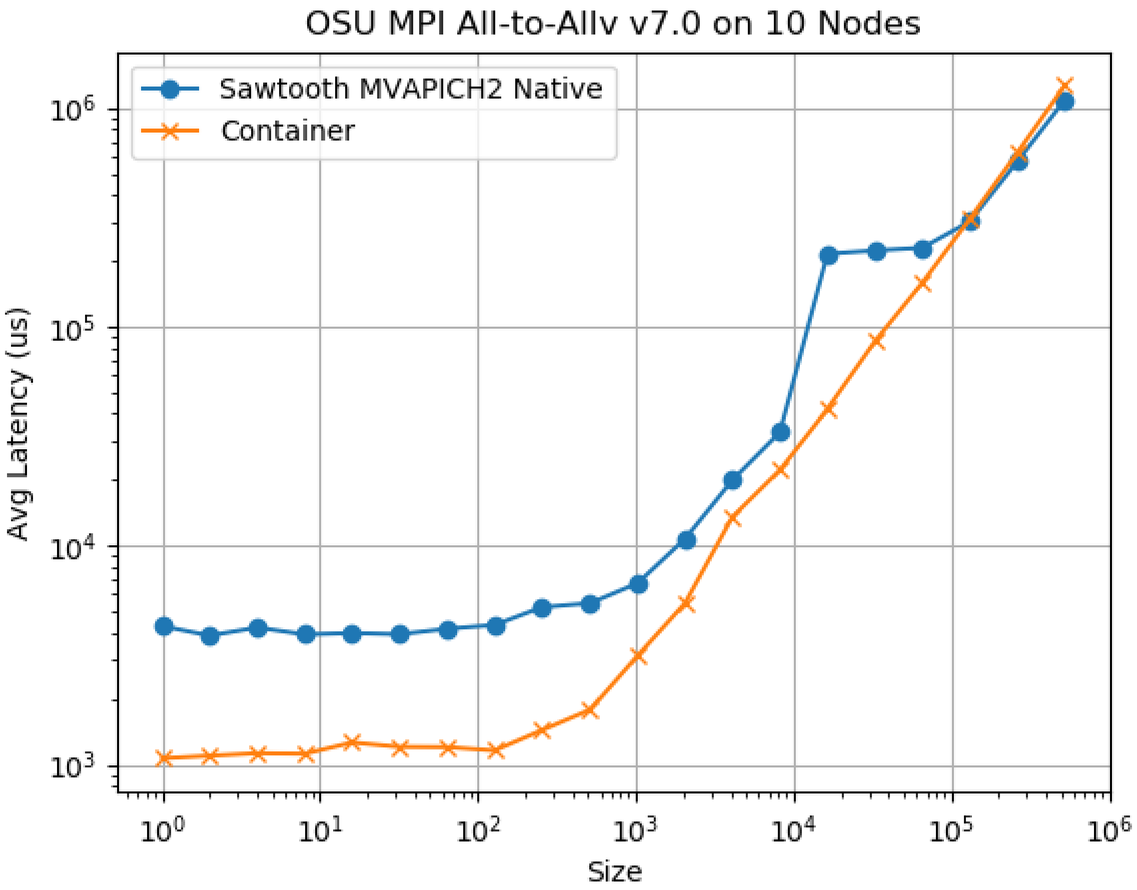


Hoodoo
OpenMPI 4.0.5

OSU MPI All-to-Allv 10 Nodes – Sawtooth

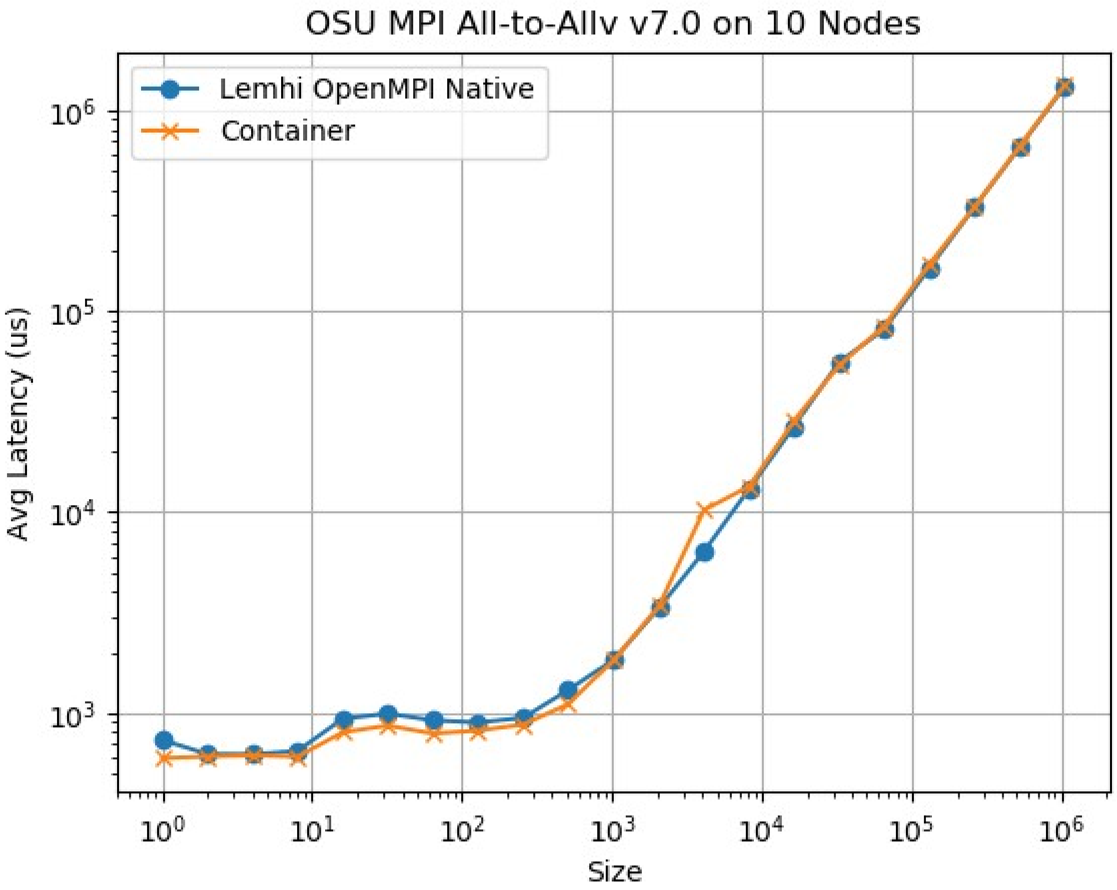


OpenMPI 4.1.4

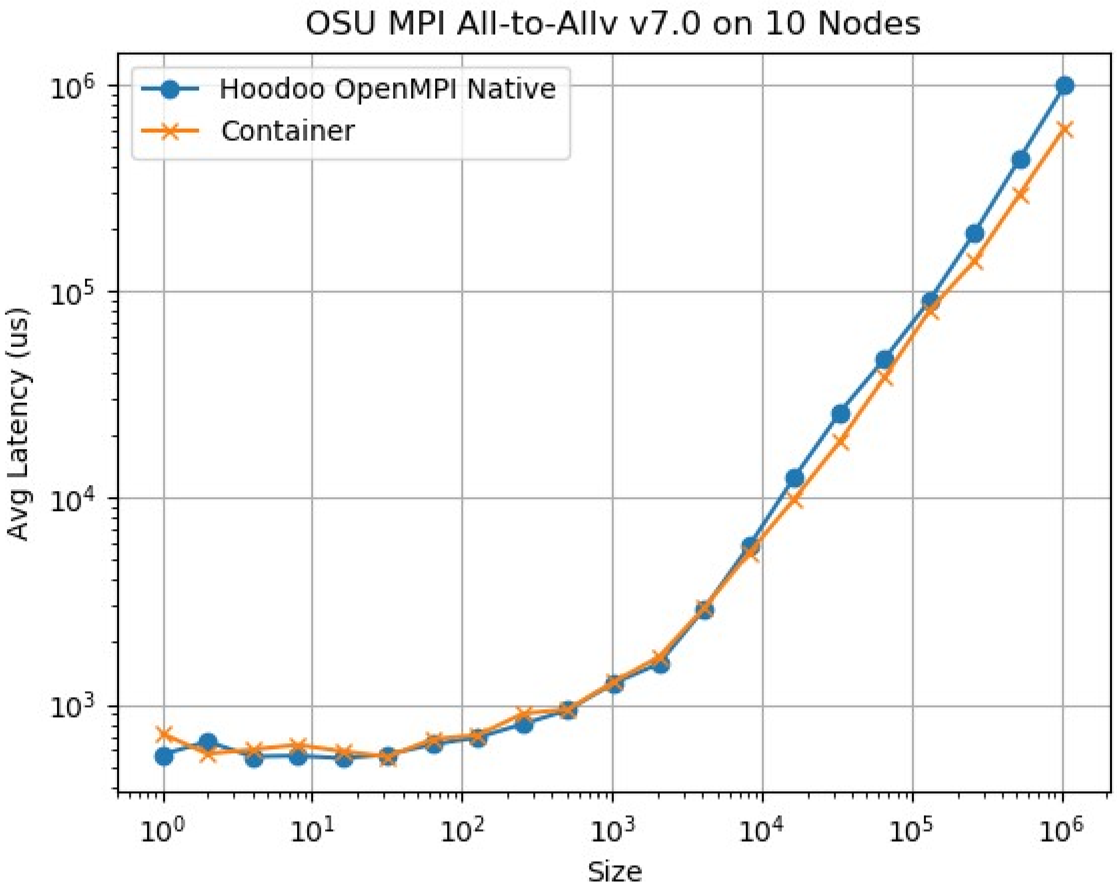


MVAPICH2 2.3.5

OSU MPI All-to-Allv 10 Nodes – Lemhi and Hoodoo

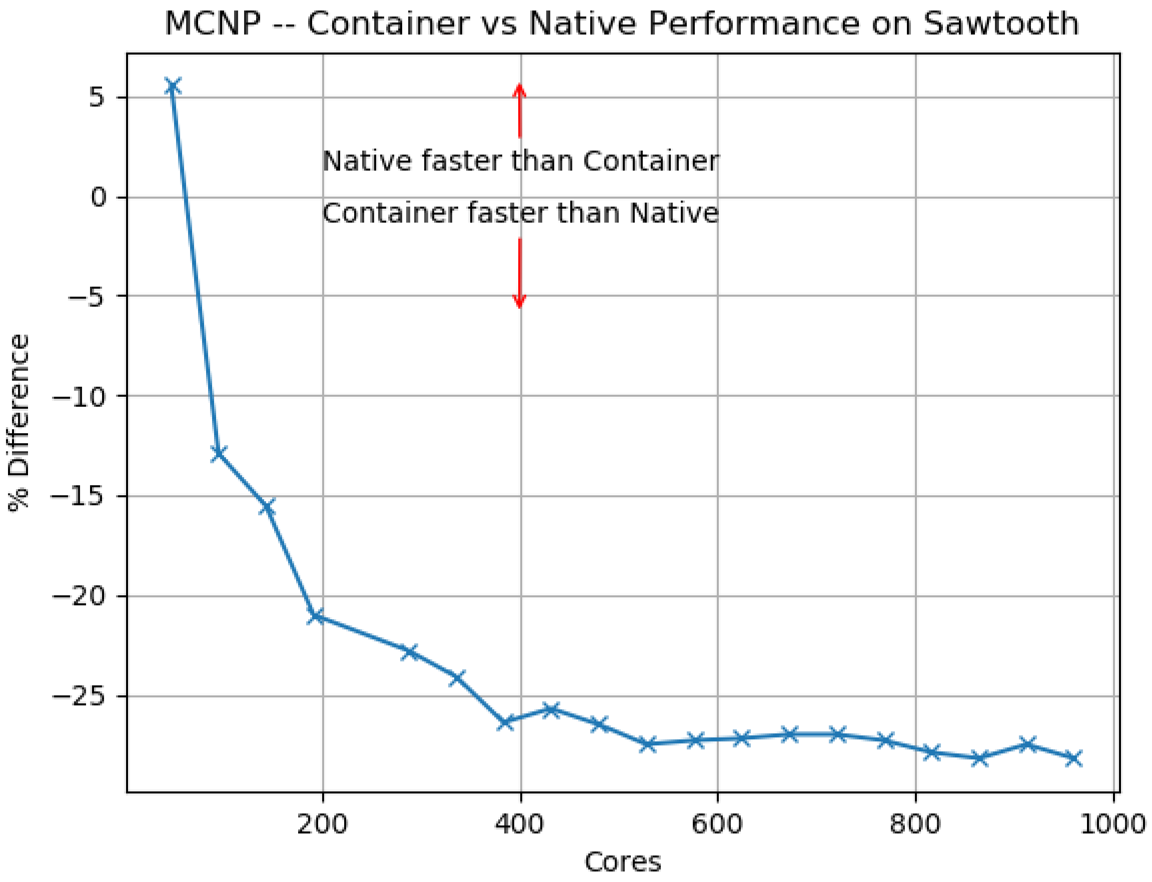


Lemhi
OpenMPI 4.1.1

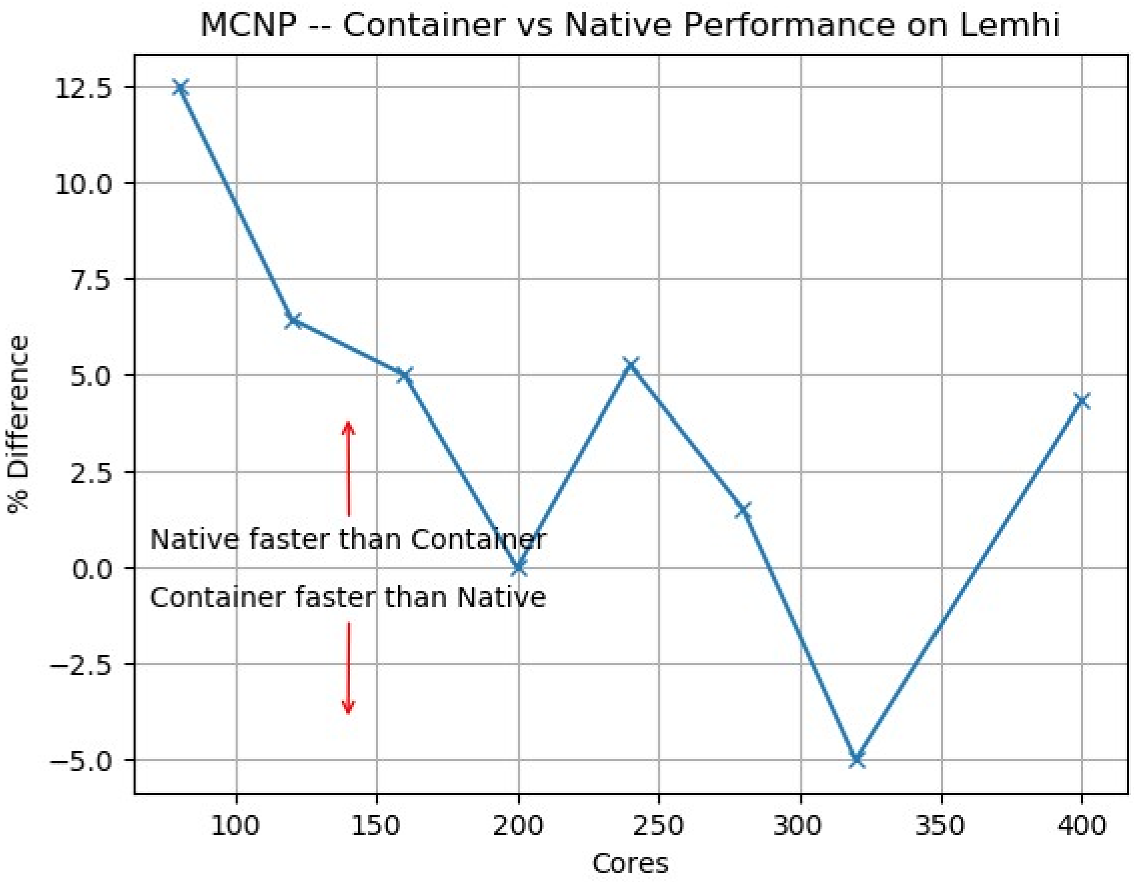


Hoodoo
OpenMPI 4.0.5

MCNP – Container vs Native Performance

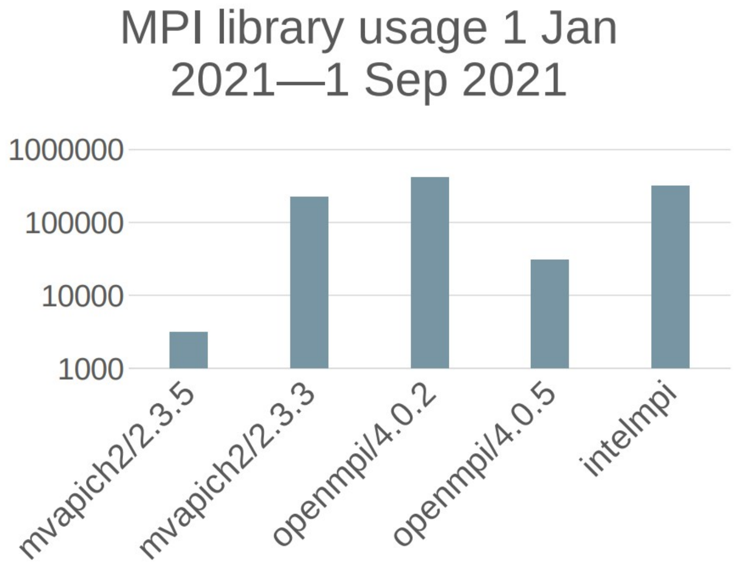


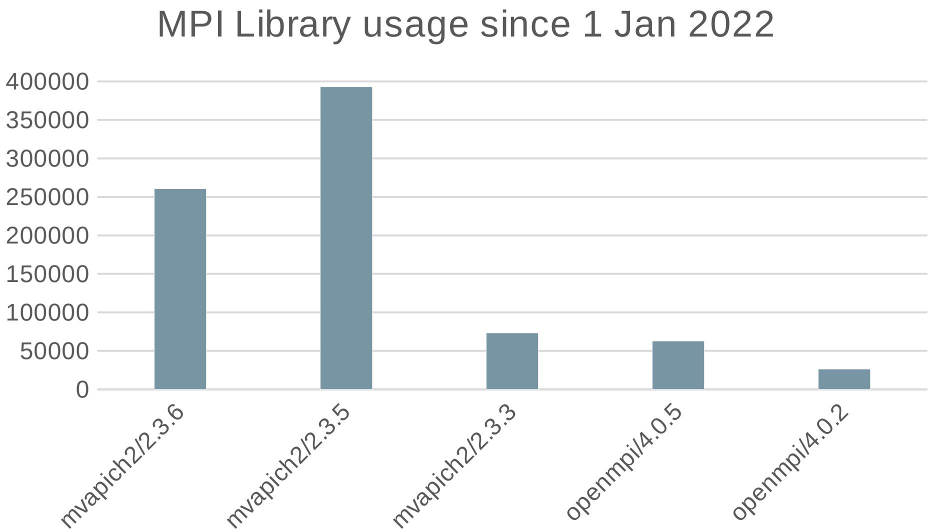
Sawtooth
OpenMPI 4.1.4

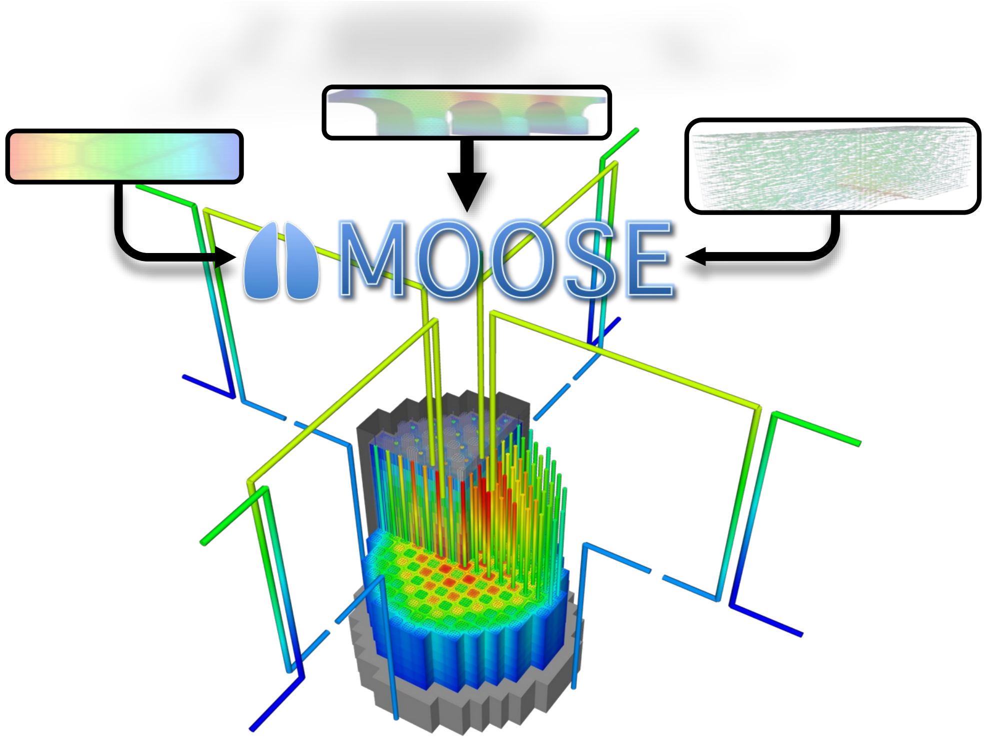


Lemhi
OpenMPI 4.1.1

MVAPICH2 and MOOSE



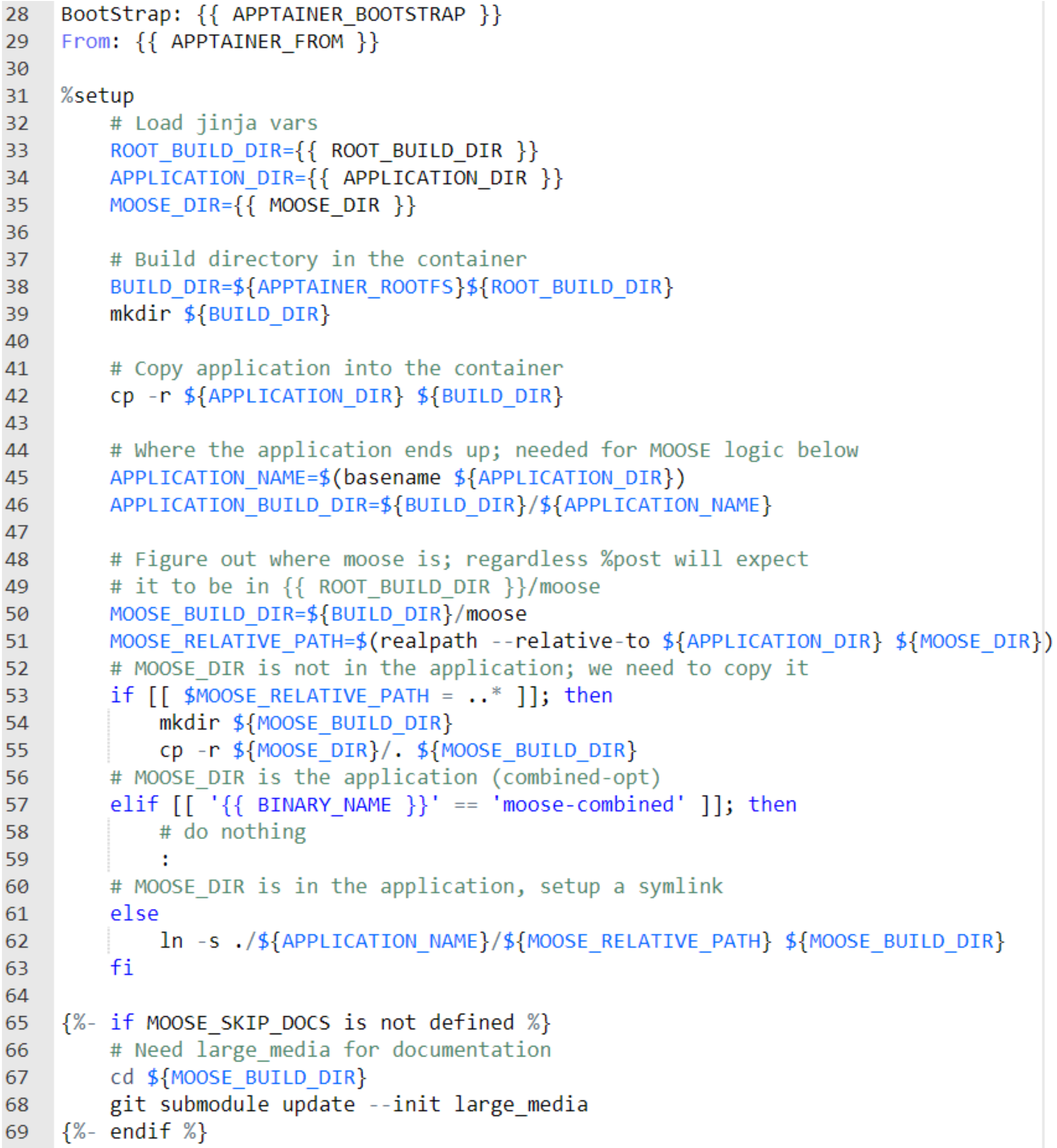




Multiphysics Object-Oriented Simulation Environment

- Open-source finite element framework
  - Basis for most nuclear modeling and simulation tools developed at INL

MOOSE Container layers – outcome



```
BootStrap: {{ APPTAINER_BOOTSTRAP }}
From: {{ APPTAINER_FROM }}

%setup
    # Load jinja vars
    ROOT_BUILD_DIR={{ ROOT_BUILD_DIR }}
    APPLICATION_DIR={{ APPLICATION_DIR }}
    MOOSE_DIR={{ MOOSE_DIR }}

    # Build directory in the container
    BUILD_DIR=${APPTAINER_ROOTFS}${ROOT_BUILD_DIR}
    mkdir ${BUILD_DIR}

    # Copy application into the container
    cp -r ${APPLICATION_DIR} ${BUILD_DIR}

    # Where the application ends up; needed for MOOSE logic below
    APPLICATION_NAME=$(basename ${APPLICATION_DIR})
    APPLICATION_BUILD_DIR=${BUILD_DIR}/${APPLICATION_NAME}

    # Figure out where moose is; regardless %post will expect
    # it to be in {{ ROOT_BUILD_DIR }}/moose
    MOOSE_BUILD_DIR=${BUILD_DIR}/moose
    MOOSE_RELATIVE_PATH=$(realpath --relative-to ${APPLICATION_DIR} ${MOOSE_DIR})
    # MOOSE_DIR is not in the application; we need to copy it
    if [[ $MOOSE_RELATIVE_PATH = ..* ]]; then
        mkdir ${MOOSE_BUILD_DIR}
        cp -r ${MOOSE_DIR}/. ${MOOSE_BUILD_DIR}
    # MOOSE_DIR is the application (combined-opt)
    elif [[ '{{ BINARY_NAME }}' == 'moose-combined' ]]; then
        # do nothing
        :
    # MOOSE_DIR is in the application, setup a symlink
    else
        ln -s ./${APPLICATION_NAME}/${MOOSE_RELATIVE_PATH} ${MOOSE_BUILD_DIR}
    fi

{%- if MOOSE_SKIP_DOCS is not defined %}
    # Need large_media for documentation
    cd ${MOOSE_BUILD_DIR}
    git submodule update --init large_media
{%- endif %}
```

- Utilizes the ”MPI + Base++” container as a base for continuous integration (non-HPC) and most HPC execution
- Improved reproducibility and portability
- Integrated into CI/CD for building workflows
  - Reduced job builds to 20 per week, which are all automated
- Simplified build process

Conclusion

- This strategy has shown the following:
  - Portability
    - Across multiple supercomputer architectures
  - Reproducibility
    - Due to layers and local mirrors
  - Traceability
    - Def files only have most recent changes
  - Simplification
    - HPC staff only needs to focus on MPI ABI and interconnect series compatibility
  - Security
    - Insulation against host system updates

Questions?

INL

Idaho National Laboratory

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