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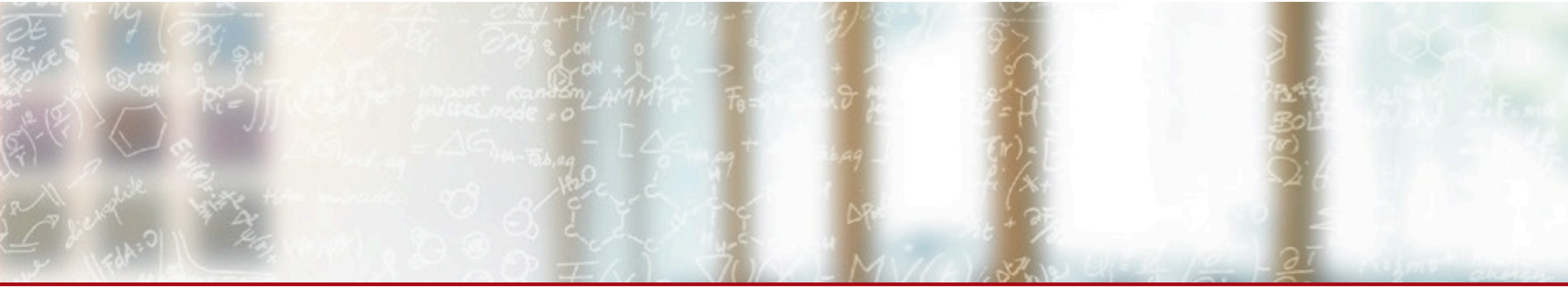

Cray Programming Environments within Containers on Cray XC Systems

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Cray User Group 2019
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Containerizing a Cray Programing Environments

- Give access to all Cray modules and software inside a container
  - Identical setup as on the production machine
  - Run on any kind of machines (non-Cray, laptop,…)

- Improve maintainability of center provided applications:
  - Prepare for next CPE: easier testing and fixing, same procedure to build
  - Increase the degree of automation for regression building
  - Assess performance evolution of applications independently of the hardware
  - Test new CPE at scale on production machine (and not only on TDS)

- Manage user expectation
  - Acknowledge increase or decrease of performance
  - Minimize compiler bugs before CPE is installed in production

Cray Programing Environments (CPE)

- A software stack to run and build application
  - Scientific libraries
  - Communication libraries
  - Compilers and variety of tools
  - External vendor packages (Intel, Nvidia,…)

- CPE is provided inside CDT ISO files
  - Version number <year>.<month>-<number> (18.10-03PRE)

- CDT contains packages
  - RPMs
  - Cray specific installer
  - CDT are tailored to a Cray system
  - Download from CrayPort

- Install packages and create modules

Container technology

- Kernel namespaces:
  - Isolate and virtualize system resources (PID, FS, network)

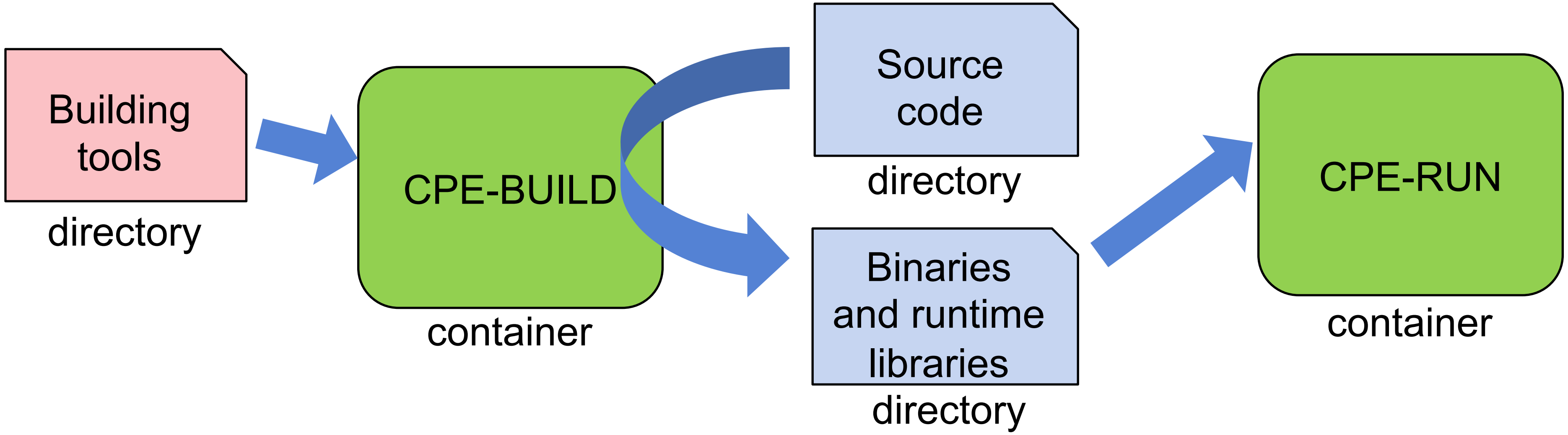
- Convenient way of packaging software stacks
  - Use a Linux distribution package manager
  - All software dependencies belong to the container
  - Kernel and drivers are outside of the container (cuda)

- Docker is the leader in container technology
  - HPC space: Singularity, Shifter, Sarus, CharlieCloud and others

CPE in container: Methodology

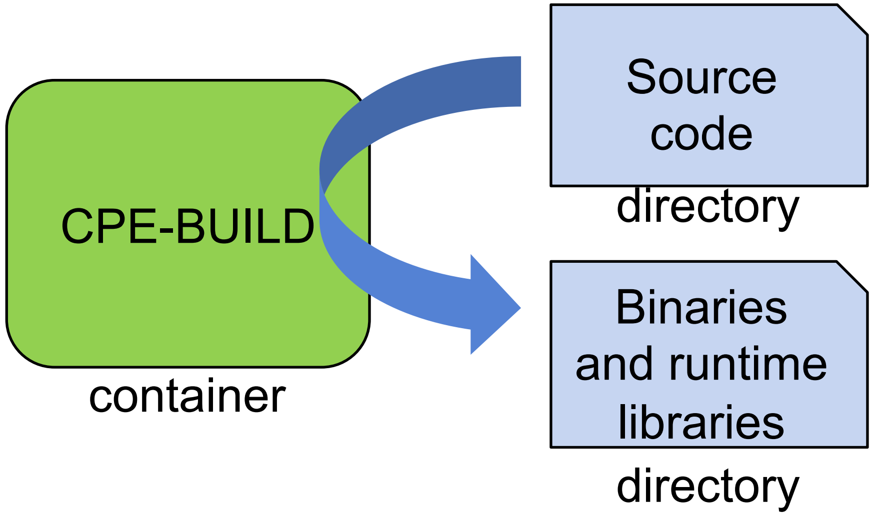
- A CPE-BUILD container can build any application
  - Input: source codes are mounted inside the container
  - Output: binaries are installed outside the container
  - One can add the required tools to build an app inside the container (easybuild,…)

- A CPE-RUN container can run an application built with a CPE-BUILD container
  - Hold the binaries and the runtime libraries
  - Special environment can be setup



CPE-BUILD

- Building the container with Docker
  - Create a Dockerfile
- Select a base image
  - Elogin node image, CLE
  - Use squashfs
- Install Cray packages
  - Configure CPE
  - Install Cray-installer
  - Install CPE
  - Install additional packages
- Setup environment
  - Input/output directories
  - Env. variables



CDT version	ISO file size	CPE container size
16.11-07	4.5 GB	34 GB
17.08-06	4.2 GB	32 GB
18.10-03	6.1 GB	50 GB

Table I
SIZE OF ISO FILE AND CPE CONTAINERS FOR VARIOUS VERSION OF CDT (INCLUDING THE CUDATOOLKIT PACKAGE).

Dockerfile(1)

Base image
Build arguments

Create user and input/output directories

Copy CDT RPMs

```
FROM elogin_prod:up07_20181205160931
ARG CDT_VERSION=18.10-03PRE
ARG CPU_TARGET=haswell
ARG ACCELERATORS=PASCAL
ARG CUDATOOLKIT=9.2

# Setup directories and pe user
RUN mkdir /root/${CDT_VERSION} && \
    mkdir /root/cuda && \
    mkdir /root/logs && \
    useradd -ms /bin/bash pe_user && \
    mkdir /home/pe_user/sources && \
    mkdir -p /home/pe_user/install/craype_runtime && \
    echo "CrayPe Version: cdt:${CDT_VERSION} cpu:${CPU_TARGET}
          acc:${ACCELERATORS} cudatoolkit:${CUDATOOLKIT}"\
       > /home/pe_user/install/craype_runtime/craype_version.txt

COPY volume/${CDT_VERSION} /root/${CDT_VERSION}
COPY cuda/ /root/cuda/
```

Dockerfile(2)

Setup and Install CDT

Install missing RPMs

Setup env.
to use modules

```
# Edit configuration and install packages
RUN cd /root/${CDT_VERSION}/installer && \
    rpm -ivh craype-installer-*.rpm --upgrade && \
    cp /opt/cray/craype-installer/default/conf/install-cdt.yaml /root && \
    sed -i -e "s/LOGS_DIR: NEED-TO-SPECIFY/LOGS_DIR : \/root\/logs/" \
        -e "s/ISO_MOUNT_DIR: NEED-TO-SPECIFY/ISO_MOUNT_DIR : \/root\/${CDT_VERSION}/" \
        -e "s/INSTALL_PGI_LIBRARIES: NO/INSTALL_PGI_LIBRARIES : YES/" \
        -e "s/INSTALL_INTEL_LIBRARIES: NO/INSTALL_INTEL_LIBRARIES : YES/" \
        -e "s/CRAY_CPU_TARGET: NEED-TO-SPECIFY/CRAY_CPU_TARGET : ${CPU_TARGET}/" \
        -e "s/ACCELERATORS: NONE/ACCELERATORS : ${ACCELERATORS}/" \
        /root/install-cdt.yaml && \
    cd /root/ && \
    /opt/cray/craype-installer/default/bin/craype-installer.pl --install \
                        --install-yaml-path install-cdt.yaml --network ari && \
    rpm -ivh /root/cuda/cray-cudatoolkit${CUDATOOLKIT}-*.rpm \
            /root/cuda/cray-nvidia-libcuda-396.44_3.1.33-6.0.7.1_3.2__gac01daf.ari.x86_64.rpm

USER pe_user
WORKDIR /home/pe_user/sources

ENV MODULEPATH /opt/cray/pe/perftools/default/modulefiles:/opt/cray/pe/craype/default/modulefiles:
            /opt/cray/pe/modulefiles:/opt/cray/modulefiles:/opt/modulefiles:/opt/cray/ari/modulefiles:
            /opt/cray/craype/default/modulefiles
```

Create base image
Import squashfs image into Docker

```
# build and import the base image
$ sudo unsquashfs -f -d unsquashfs elogin_prod_up07_20181205160931.squashfs
$ sudo tar -C unsquashfs -c . | docker import - elogin_prod:up07_20181205160931
```

Directory structure and file locations

```
# directory structure
$ ls .
Dockerfile cuda volume

$ ls cuda/
cray-cudatoolkit8.0-8.0.61_2.4.9-6.0.7.0_17.1__g899857c.x86_64.rpm
cray-cudatoolkit9.0-9.0.103_3.15-6.0.7.0_14.1__ge802626.x86_64.rpm
cray-cudatoolkit9.2-9.2.148_3.19-6.0.7.1_2.1__g3d9acc8.x86_64.rpm
cray-nvidia-libcuda-390.46_3.1.30-6.0.7.0_24.8__g83596c3.ari.x86_64.rpm
cray-nvidia-libcuda-396.44_3.1.33-6.0.7.1_3.2__gac01daf.ari.x86_64.rpm

$ ls volume/16.11-07/
TRANS.TBL    conf    docs    installer    packages    release_info
```

Build the container with build arguments

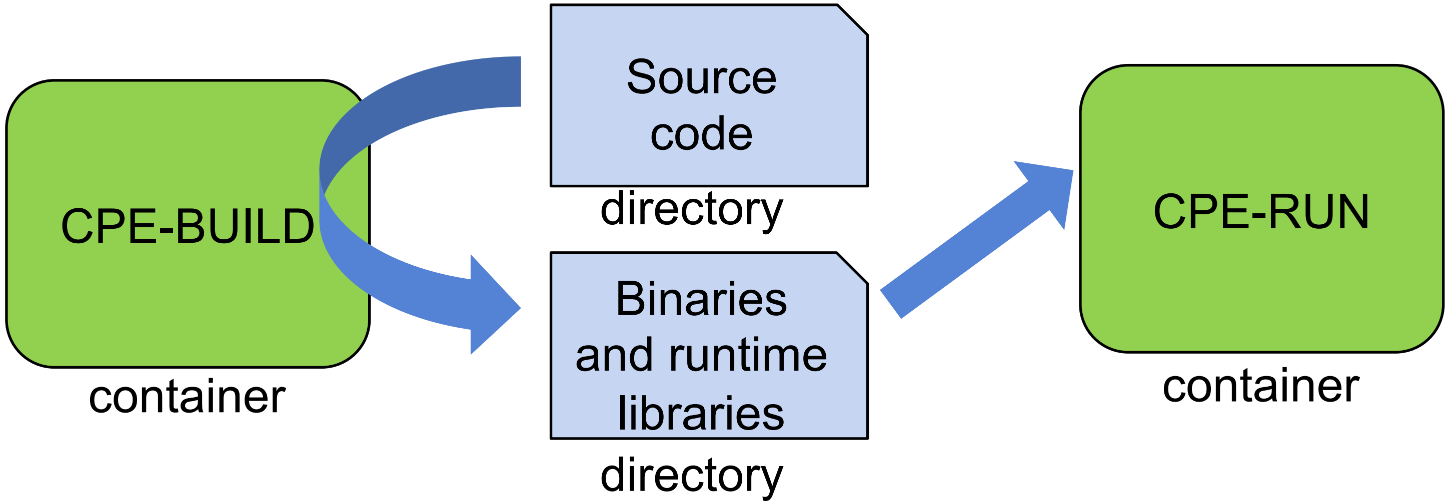
```
$ docker build --build-arg CDT_VERSION=16.11-07 --build-arg CUDATOOLKIT=8.0 \
        -t craype:cdt16.11-07.haswell.pascal.cudatoolkit8.0 .
```

Start interactively the CPE-BUILD, set input and output directories

```
$ docker run -v /Users/maximem/dev/docker/my_source:/home/pe_user/sources \
        -v /Users/maximem/dev/pe_container/my_binaries:/home/pe_user/install \
        --rm -it craype:cdt16.11-07.haswell.pascal.cudatoolkit8.0 /bin/bash
```

CPE-RUN: Lightweight container

- Compiled binary
  - Outside of container
  - Dependency inside container
- Extract dependencies
  - Python script *ldd* and *strings*
  - Lookup for *dlsym* libraries



- Binaries and dependencies are inside one directory outside of CPE-BUILD
  - Option 1: Copy directory, set *LD_LIBRARY_PATH* and run
  - Option 2: Copy inside a lightweight container with proper env. setup

Example of script output

```
$ ldd_parser --binaries /opt/cray/pe/cce/8.7.3/cce/x86_64/lib/libfi.so
/opt/cray/pe/gcc-libs/libstdc++.so.6
/opt/cray/pe/gcc-libs/libgfortran.so.3
/opt/cray/pe/cce/8.7.3/cce/x86_64/lib/libf.so.1
/opt/cray/pe/cce/8.7.3/cce/x86_64/lib/libcsup.so.1
/opt/cray/pe/cce/8.7.3/cce/x86_64/lib/libu.so.1
/opt/cray/pe/cce/8.7.3/cce/x86_64/lib/libcraymath.so.1
# Duplicated reference of libraries:
/opt/cray/pe/cce/8.7.3/cce/x86_64/lib/libquadmath.so.0
/opt/gcc/6.2.0/snos/lib/../lib64/libquadmath.so.0
/opt/cray/pe/gcc-libs/libgcc_s.so.1
/opt/gcc/6.2.0/snos/lib/../lib64/libgcc_s.so.1
# dlsym libraries:
libmemkind.so.0
libnuma.so
```

Limitations and challenges

- There is a variability in installed packages depending on the CDT version
  - Getting more regular with later CDT versions
  - Not all packages are installed
  - Might need a Dockerfile per CDT version

- Cuda and drivers
  - Careful which version of the driver is installed, backward compatibility works
  - Forward compatibility: cuda10

- Identifying dependencies
  - Not automated, need a human in the loop to check script output

- Built binaries should run on a Cray system
  - Careful with the license agreement

Use case: Reproducible experiments

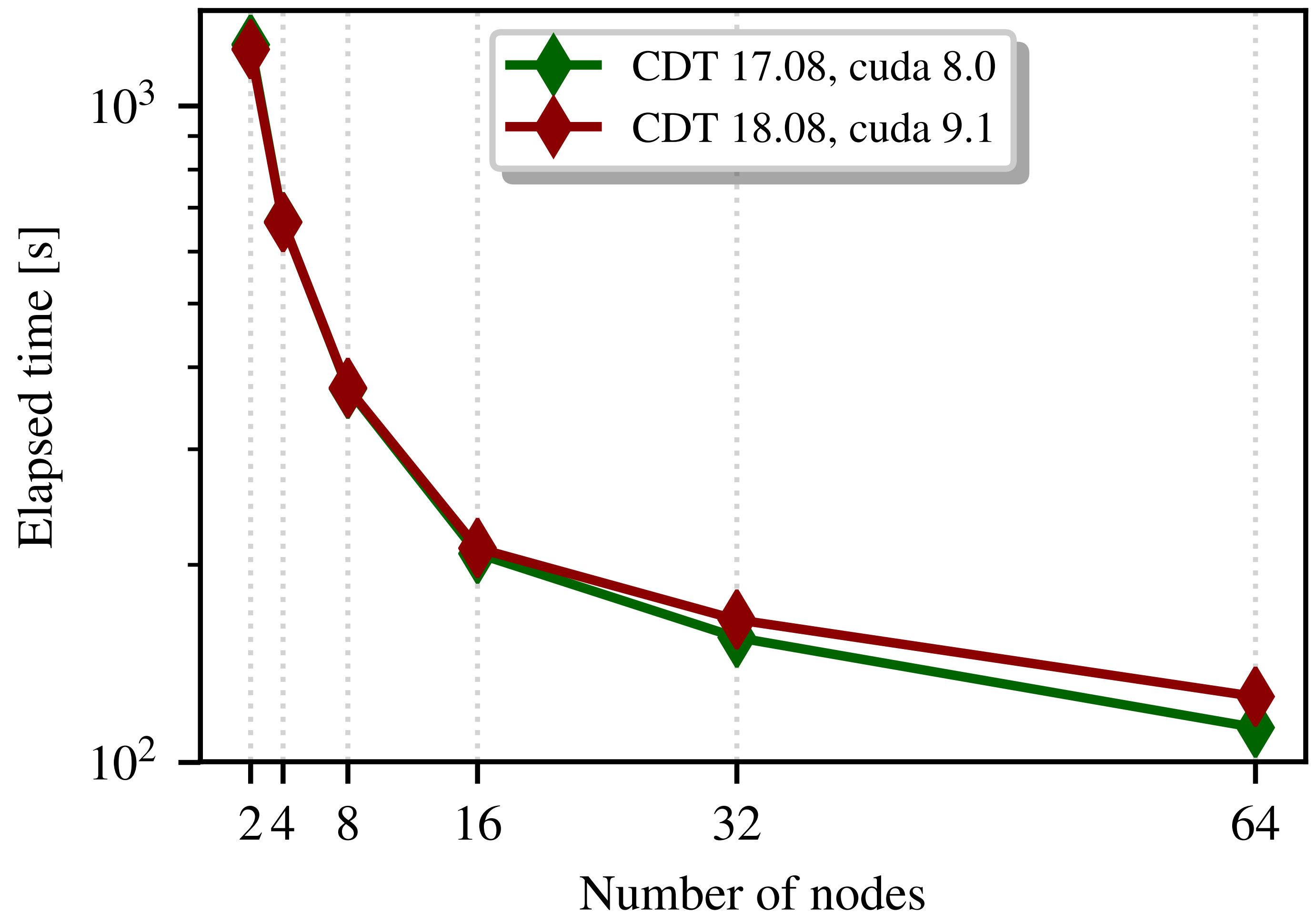
- Institute for Atmospheric and Climate Science
  - COSMO: weather and climate application that has been ported to GPU
  - COSMO: Fortran + OpenACC and C++ with Cuda
  - COSMO-OPCODE version: no major update since 2015
  - Ensure reproducible experiments over 2 to 4 years time due to publication requirements

- Built with CDT 16.11 at the time of publication
  - Consume a large effort to update COSMO-OPCODE to new CPE
  - Current is 18.09, does not compile with CCE > 8.5.5, no resource to investigate
  - Install CDT 16.11 on Piz Daint (number of deployed CPEs, image size)

- Reproducibility, built within a container and run on Piz Daint
  - It passes the COSMO-OPCDE test suite
  - Produces a "useful climate”? (expert to check)

Use case: Performance variability

- CP2K built with 2 CPEs
  - 17.08 Cuda 8.0
  - 18.08 Cuda 9.1
- Standard benchmarks
  - H2O_256
  - 1 MPI +12 OpenMP / node
  - Piz Daint, 12 cores, P100
- CDT 17.08 scales better
  - 10% faster at 64 nodes
  - Was MPI getting slower?



Conclusion

- CPE in container is easy and helpful
  - Same procedure to install CPEs
  - No extra requirements on the container technology

- Should Cray provide containers instead of CDT iso files?
- Should Cray provide a package manager to use inside a Dockerfile?

- Open a build service with containerized CPEs to users?
  - Maintain multiple CPEs per applications
  - Easy integration with various building tools

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Thank you for your attention.