Containerization of simulation applications for frequently re-run configurations

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BACKGROUND

Motivation

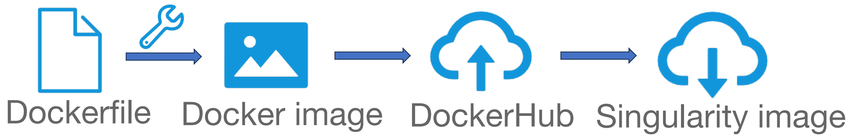
The Complexity of software makes it difficult to build, install and run on different architectures.

Container makes the software both shareable and portable while the output becomes reproducible.

Goal

This project focus on using Singularity containers to automate the compilation process of a scientific simulation CM1 with various MPI and GPU versions.

SOLUTION



Docker

- Use **Spack** to install compilers and packages

```
FROM centos:7.8.2003

RUN git clone -c feature.manyFiles=true
https://github.com/spack/spack.git /home/spack && \
. /home/spack/share/spack/setup-env.sh && \
CXX=g++ && CC=gcc && FC=gfortran && \
spack install nvhpc@22.2 %gcc@9.3.1

ENV PATH="/home/spack/bin:$PATH"
```

- Use **multi-stage** build to shrink the container size

```
FROM meditates/cm1:spack3 AS builder
FROM centos:7.8.2003 AS production
WORKDIR /home
COPY --from=builder /home/spack/opt/spack/linux-centos7-
skylake_avx512/oneapi-2021.4.0/openmpi-4.1.5-
apagapfdf7jtq2eruixznynciu5lyqjw/lib/libmpi_usempif08.so.40 /lib64
```

Spack Package manager

Singularity

Container platform for HPC

- Build from Docker images

$ singularity build **--fix-perms** cm1_spack.sif docker://meditates/cm1:spack

- Build application CM1

$ singularity exec **--nv --bind /glade/:/glade** cm1_spack.sif intel-openmpi.sh

- Submit a CM1 job (qcmd is for an interactive job submission)

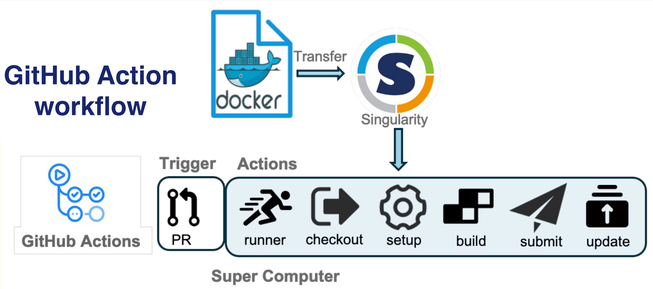
$ qcmd -q casper -l select=1:ncpus=2:mpiprocs=2 -A <myaccount> -l walltime=3:00:00 -- "submit_intel.sh"

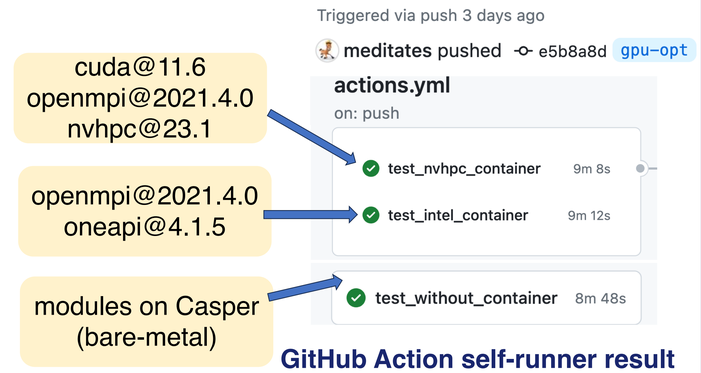
VALIDATION

myCM1/github/workflows/actions.yml

```
name: Container Project
on:
  push:
    branches:
      - gpu-opt
env:
  PLATFORM: casper
jobs:
  test_intel_container:
    runs-on: self-hosted
    steps:
    - name: Check out repository code
      uses: actions/checkout@v3
    - name: build
      working-directory: ${{github.workspace}}/src
      run: |
        module load singularity
        …..
    - name: run with input
```

GitHub Action workflow





GitHub Action self-runner result

CHALLENGES

Spack:
- Some dependency packages need to set basic compiler in the spack compiler yaml file.
- Environment variable setting.
- Network not stable, slow install speed.

Docker:
- Compatibility between base image and package.

Singularity:
- Slow image build speed.
- Proper command to submit job to Casper.

GitHub Action:
- Security concern.

FUTURE WORK

- Build more general containers that can run both on Casper and Derecho.
- Experiment with multiple mpich and nvhpc versions on containers.
- Validate and compare the result of different containers.

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