

Run MPI with containers

Simple test

Simple container with ucx and openmpi.

Bootstrap: docker

From: debian:trixie

%environment

```
export LD_LIBRARY_PATH=/usr/local/lib
```

%post

```
apt-get update && apt-get install -y build-essential wget rdma-core libibverbs-dev
```

```
wget https://github.com/openucx/ucx/releases/download/v1.18.1/ucx-1.18.1.tar.gz
```

```
tar xzf ucx-1.18.1.tar.gz
```

```
cd ucx-1.18.1
```

```
mkdir build
```

```
cd build
```

```
./configure --prefix=/opt/
```

```
make -j4
```

```
make install
```

```
cd ..
```

```
export OPENMPI_VERSION="4.1.6"
```

```
export OPENMPI_MAJOR_VERSION="v4.1"
```

```
export OPENMPI_MAKE_OPTIONS="-j4"
```

```
mkdir -p /openmpi-src
```

```
cd /openmpi-src
```

```
wget https://download.open-mpi.org/release/open-mpi/${OPENMPI_MAJOR_VERSION}/openmpi-${OPENMPI_VERSION}.tar.gz \
```

```
&& tar xzf openmpi-${OPENMPI_VERSION}.tar.gz
```

```
cd openmpi-${OPENMPI_VERSION} && ./configure --with-ucx=/opt
```

```
make all ${OPENMPI_MAKE_OPTIONS}
```

```
make install
```

```
cd /
```

```
rm -rf /openmpi-src
```

To build it:

```
singularity build -f openmpitest.sif openmpi.def
```

Then we compile an MPI application inside the container. For example [osu-benchmarks](#).

```
wget https://mvapich.cse.ohio-state.edu/download/mvapich/osu-micro-benchmarks-7.5-1.tar.gz
tar -xvf osu-micro-benchmarks-7.5-1.tar.gz
```

```
singularity shell openmpitest.sif
```

```
cd osu-micro-benchmarks-7.5-1
./configure CC=/usr/local/bin/mpicc CXX=/usr/local/bin/mpicxx --prefix=/scratch/$user/osu_install
make install
```

Then you can use the following job:

```
#!/bin/bash

#SBATCH -N 2
#SBATCH -n 2
#SBATCH -o mpi-%j.out
#SBATCH -e mpi-%j.err

module purge
module load singularityce
module load openmpi

export SINGULARITY_BINDPATH=/usr/lib64/libmunge.so.2,/var/run/munge,/scratch

srun --mpi=pmix singularity run openmpitest.sif /scratch/$user/osu-install/libexec/osu-micro-
benchmarks/mpi/collective/osu_alltoall
```

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Créé 19 mai 2025 11:09:14 par Cristian Ruiz

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