Installation procedure of openmpi with CUDA support on BioHPC – Please do this on a GPU node with V100s or A100 GPU:

```
cd /path/to/where/you/want/to/install/

# Download the openmpi from the official website
wget https://download.open-mpi.org/release/open-mpi/v3.0/openmpi-3.0.0.tar.gz

# Extract files and create a "build folder"
tar -xvzf openmpi-3.0.0.tar.gz
cd openmpi-3.0.0
mkdir build

# At this point, your path looks like /path/to/where/you/want/to/install/openmpi-3.0.0
- Then follow the procedure below to install openmpi

module load gcc/6.3.0

./configure --prefix=/path/to/where/you/want/to/install/openmpi-3.0.0/build --with-knem=/opt/knem-1.1.3.90mlnx1  --with-verbs --with-ucx --with-slurm=/cm/shared/apps/slurm/current --with-pmi=/cm/shared/apps/slurm/current --with-cuda=/cm/shared/apps/cuda112/toolkit/11.2.0/include

make -j32

make install
```