

Open MPI 4.1.6

Webpage

<https://www.open-mpi.org/>

Version

- 4.1.6

Build Environment

- gcc 8.5.0, 11.2.1, 12.1.1
- Intel oneAPI Compiler Classic 2022.2.1, 2023.2.0
- Intel oneAPI Compilers 2023.2.0
- AOCC 4.1
- NVIDIA HPC SDK 23.5

- OpenPBS 22.05.11

Files Required

- openmpi-4.1.6.tar.bz2

Build Procedure

gcc 8, 11, 12

```
#!/bin/sh

VERSION=4.1.6
WORKDIR=/gwork/users/${USER}
TARBALL=/home/users/${USER}/Software/OpenMPI/${VERSION}/openmpi-${VERSION}.tar.bz2
PBSROOT=/apl/pbs/22.05.11

PARALLEL=12

#-----
umask 0022

cd ${WORKDIR}
if [ -d openmpi-${VERSION} ]; then
  mv openmpi-${VERSION} openmpi-erase
  rm -rf openmpi-erase &
fi

tar jxf ${TARBALL}
cd openmpi-${VERSION}

# GCC 8
module purge
INSTALLDIR=/apl/openmpi/${VERSION}/gcc8
mkdir rccs-gcc8 && cd rccs-gcc8
../configure --prefix=${INSTALLDIR} \
  --with-tm=${PBSROOT} \
  --enable-mpi-cxx \
  --with-ucx \
  --enable-mpi1-compatibility
make -j ${PARALLEL} && make install && make check
cd ../

# GCC 11
module purge
module load gcc-toolset/11
```

```

INSTALLDIR=/apl/openmpi/${VERSION}/gcc11
mkdir rccs-gcc11 && cd rccs-gcc11
../configure --prefix=${INSTALLDIR} \
    --with-tm=${PBSROOT} \
    --enable-mpi-cxx \
    --with-ucx \
    --enable-mpi1-compatibility
make -j ${PARALLEL} && make install && make check
cd ../

```

```
# GCC 12
```

```
module purge
```

```
module load gcc-toolset/12
```

```
INSTALLDIR=/apl/openmpi/${VERSION}/gcc12
```

```
mkdir rccs-gcc12 && cd rccs-gcc12
```

```
../configure --prefix=${INSTALLDIR} \
```

```
    --with-tm=${PBSROOT} \
```

```
    --enable-mpi-cxx \
```

```
    --with-ucx \
```

```
    --enable-mpi1-compatibility
```

```
make -j ${PARALLEL} && make install && make check
```

```
cd ../
```

intel 2022 (classic)

```
#!/bin/sh
```

```
VERSION=4.1.6
```

```
WORKDIR=/gwork/users/${USER}
```

```
TARBALL=/home/users/${USER}/Software/OpenMPI/${VERSION}/openmpi-${VERSION}.tar.bz2
```

```
PBSROOT=/apl/pbs/22.05.11
```

```
PARALLEL=12
```

```
# -----
```

```
umask 0022
```

```
cd ${WORKDIR}
```

```
if [ -d openmpi-${VERSION} ]; then
```

```
    mv openmpi-${VERSION} openmpi-erase
```

```
    rm -rf openmpi-erase &
```

```
fi
```

```
tar jxf ${TARBALL}
```

```
cd openmpi-${VERSION}
```

```
# intel compiler classic 2022.2.1
```

```
module purge
```

```
. ~/intel/oneapi/compiler/2022.2.1/env/vars.sh
```

```
export CC=icc
```

```
export CXX=icpc
```

```
export FC=ifort
```

```
INSTALLDIR=/apl/openmpi/${VERSION}/intel2022
```

```
mkdir rccs-intel && cd rccs-intel
```

```
../configure --prefix=${INSTALLDIR} \
```

```
    --with-tm=${PBSROOT} \
```

```
    --enable-mpi-cxx \
```

```
    --with-ucx \
```

```
    --enable-mpi1-compatibility
```

```
make -j ${PARALLEL} && make install && make check
```

```
cd ../
```

intel 2023 (classic)

```

#!/bin/sh

VERSION=4.1.6
WORKDIR=/gwork/users/${USER}
TARBALL=/home/users/${USER}/Software/OpenMPI/${VERSION}/openmpi-${VERSION}.tar.bz2
PBSROOT=/apl/pbs/22.05.11

PARALLEL=12

#-----
umask 0022

cd ${WORKDIR}
if [ -d openmpi-${VERSION} ]; then
  mv openmpi-${VERSION} openmpi-erase
  rm -rf openmpi-erase &
fi

tar jxf ${TARBALL}
cd openmpi-${VERSION}

# intel compiler classic 2023.2.0
module purge
. ~/intel/oneapi/compiler/2023.2.0/env/vars.sh

export CC=icc
export CXX=icpc
export FC=ifort

INSTALLDIR=/apl/openmpi/${VERSION}/intel2023
mkdir rccs-intel && cd rccs-intel
./configure --prefix=${INSTALLDIR} \
  --with-tm=${PBSROOT} \
  --enable-mpi-cxx \
  --with-ucx \
  --enable-mpi1-compatibility
make -j ${PARALLEL} && make install && make check
cd ../

```

intel 2023

```

#!/bin/sh

VERSION=4.1.6
WORKDIR=/gwork/users/${USER}
TARBALL=/home/users/${USER}/Software/OpenMPI/${VERSION}/openmpi-${VERSION}.tar.bz2
PBSROOT=/apl/pbs/22.05.11

PARALLEL=12

#-----
umask 0022

cd ${WORKDIR}
if [ -d openmpi-${VERSION} ]; then
  mv openmpi-${VERSION} openmpi-erase
  rm -rf openmpi-erase &
fi

tar jxf ${TARBALL}
cd openmpi-${VERSION}

# intel compiler icx/icpx 2023.2.0
module purge
. ~/intel/oneapi/compiler/2023.2.0/env/vars.sh

```

```

export CC=icx
export CXX=icpx
export FC=ifx

INSTALLDIR=/apl/openmpi/${VERSION}/intel2023-icx
mkdir rccs-intel && cd rccs-intel
./configure --prefix=${INSTALLDIR} \
    --with-tm=${PBSROOT} \
    --enable-mpi-cxx \
    --with-ucx \
    --enable-mpi1-compatibility
make -j ${PARALLEL} && make install && make check
cd ../

```

aocc 4.1

```

#!/bin/sh

VERSION=4.1.6
WORKDIR=/gwork/users/${USER}
TARBALL=/home/users/${USER}/Software/OpenMPI/${VERSION}/openmpi-${VERSION}.tar.bz2
PBSROOT=/apl/pbs/22.05.11

PARALLEL=12

#-----
umask 0022

cd ${WORKDIR}
if [ -d openmpi-${VERSION} ]; then
    mv openmpi-${VERSION} openmpi-erase
    rm -rf openmpi-erase &
fi

tar jxf ${TARBALL}
cd openmpi-${VERSION}

# AOCC 4.1.0
module -s purge
module -s load aocc/4.1.0

export CC=clang
export CXX=clang++
export FC=flang

INSTALLDIR=/apl/openmpi/${VERSION}/aocc4.1
mkdir rccs-aocc41 && cd rccs-aocc41
./configure --prefix=${INSTALLDIR} \
    --with-tm=${PBSROOT} \
    --enable-mpi-cxx \
    --with-ucx \
    --without-libfabric \
    --enable-mpi1-compatibility
make -j ${PARALLEL} && make install && make check
cd ../

```

nvidia hpc sdk 23.5

```

#!/bin/sh

VERSION=4.1.6
WORKDIR=/gwork/users/${USER}
TARBALL=/home/users/${USER}/Software/OpenMPI/${VERSION}/openmpi-${VERSION}.tar.bz2
PBSROOT=/apl/pbs/22.05.11

```

```
PARALLEL=12

#-----
umask 0022

cd ${WORKDIR}
if [ -d openmpi-${VERSION} ]; then
  mv openmpi-${VERSION} openmpi-erase
  rm -rf openmpi-erase &
fi

tar jxf ${TARBALL}
cd openmpi-${VERSION}

# nvidia hpc sdk 22.11
module purge
module load nvhpc/23.5-nompi

export CC=nvc
export CXX=nvc++
export FC=nvfortran

export CFLAGS="-fPIC"
export CXXFLAGS="-fPIC"
export FCFLAGS="-fPIC"
export LDFLAGS="-fPIC"

export CUDA_HOME=${NVHPC_ROOT}/cuda

INSTALLDIR=/apl/openmpi/${VERSION}/nv23
mkdir rccs-nv23 && cd rccs-nv23
./configure --prefix=${INSTALLDIR} \
  --with-tm=${PBSROOT} \
  --enable-mpi-cxx \
  --with-ucx \
  --with-cuda=${CUDA_HOME} \
  --enable-mpi1-compatibility
make -j ${PARALLEL} && make install && make check
cd ../
```