

PSI4-1.10

Webpage

<https://psicode.org/>

Version

1.10

Build Environment

- miniforge environment will be installed in the procedure below
 - python 3.12.12
 - GCC 14.3.0 (gcc, g++, gfortran)
 - cmake 4.2.0

Files Required

- (files will be downloaded during installation)

Build Procedure

```
#!/bin/sh

VERSION=1.10
INSTALL_DIR=/apl/psi4/${VERSION}
PSI4_URL=https://github.com/psi4/psi4.git

WORKDIR=/gwork/users/${USER}

MINIFORGE_VERSION=25.9.1-0
MINIFORGE_ARCH=Linux-x86_64
MINIFORGE=Miniforge3-${MINIFORGE_VERSION}-${MINIFORGE_ARCH}.sh
MINIFORGE_URL=https://github.com/conda-
forge/miniforge/releases/download/${MINIFORGE_VERSION}/${MINIFORGE}

export LANG=C
PARALLEL=12

# -----
umask 0022

module -s purge
module -s load pbs/22.05.11
```

```
cd ${INSTALL_DIR}
wget ${MINIFORGE_URL}
sh ${MINIFORGE} -b -p ${INSTALL_DIR}/miniforge3
${INSTALL_DIR}/miniforge3/bin/conda shell.bash hook > ${INSTALL_DIR}/conda_init.sh
${INSTALL_DIR}/miniforge3/bin/conda shell.tcsh hook > ${INSTALL_DIR}/conda_init.csh
. ${INSTALL_DIR}/conda_init.sh
rm -f ${MINIFORGE} wget-log
```

```
cd ${WORKDIR}
if [ -d psi4 ]; then
  mv psi4 psi4-erase
  rm -rf psi4-erase &
fi
git clone -b v${VERSION} ${PSI4_URL}
cd psi4
conda/psi4-path-advisor.py env --python 3.12 --name base --disable addons docs
conda env update --file env_base.yaml
conda install -y regex jsonschema doxygen geometric gcp-correction \
  zlib fortran-compiler pylibfp armadillo \
  unicode dftd3-python dftd4-python
```

```
export CMAKE_POLICY_VERSION_MINIMUM=3.5
mkdir build && cd build
```

```
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_DIR} \
  -DBUILD_SHARED_LIBS=ON \
  -DCMAKE_C_COMPILER=gcc \
  -DCMAKE_CXX_COMPILER=g++ \
  -DCMAKE_Fortran_COMPILER=gfortran \
  -DENABLE_CheMPS2=ON \
  -DENABLE_Einsums=ON \
  -DENABLE_IntegratorXX=ON \
  -DENABLE_OpenOrbitalOptimizer=ON \
  -DENABLE_PCMSolver=ON \
  -DENABLE_adcc=OFF \
  -DENABLE_ambit=ON \
  -DENABLE_bse=ON \
  -DENABLE_ccsort=OFF \
  -DENABLE_cct3=ON \
  -DENABLE_cppe=ON \
  -DENABLE_ddx=ON \
  -DENABLE_dkh=ON \
  -DENABLE_ecpint=ON \
  -DENABLE_gdma=ON \
  -DENABLE_libfp=ON \
  -DENABLE_mdi=ON \
  -DENABLE_psi4fockci=ON \
  -DENABLE_simint=ON \
```

```
-DENABLE_snsmp2=OFF \  
-DENABLE_transqt2=OFF \  
-DENABLE_v2rdm_casscf=ON  
make -j ${PARALLEL}  
make install  
  
export PATH=${INSTALL_DIR}/bin:${PATH}  
export LD_LIBRARY_PATH=${INSTALL_DIR}/lib:${LD_LIBRARY_PATH}  
export PYTHONPATH=${INSTALL_DIR}/lib:${PYTHONPATH}  
  
ctest -j${PARALLEL}  
mkdir -p ${INSTALL_DIR}/test_results  
cp Testing/Temporary/* ${INSTALL_DIR}/test_results
```

Tests

All the tests have passed successfully. Copy of test log is available in /apl/psi4/1.10/test_results.

Notes

- If compilers from gcc-toolset were employed, mcsf2 test failed.
 - Gcc-toolset 11, 12, and 14 were tested. Gcc-toolset 13 was not tested. (Most probably gcc-toolset 13 compilers may be failed, too.) This can be attributed to common runtime library in /usr/lib64. (not investigated)
- "export CMAKE_POLICY_VERSION_MINIMUM=3.5" line may be necessary if cmake 4.x is employed.
- adcc, ccsort, transqt2 were disabled to avoid compilation error.
 - There is no build issue for snsmp2. However, it puts warning message upon launch and all the snsmp2 tests have failed.
- Intel Compiler (LLVM) can build psi4 without significant problem (some of optional packages should be disabled). However, parallel performance of intel version is slightly lower than that of gcc version on RCCS system.