

PSI4 1.7

Webpage

<https://psicode.org/>

Version

1.7

Build Environment

- Intel oneAPI Compiler Classic 2022.2.1
- Intel MKL 2022.2.1
- boost 1.81.0
- (Python 3.10.8 (miniforge3))

Files Required

- psi4.tar.gz
 - manually archived directory after git checkout refs/tags/v1.7
- libint-2.7.2.tar.gz
- (some of files are downloaded in the procedure below)
- (CheMPS2 was obtained by git command)

Build Procedure

conda environment (miniforge)

Lost detailed procedure. Basically the same procedure as [1.5 case](#), while scipy is additionally installed and rdkit is not installed. (according to the memo)

CheMPS2

Lost detailed procedure. Basically the same procedure as [1.5 case](#) using Intel Compilers and MKL. (according to the memo)

libint-2.7.2 (brief summary)

```
$ . ~/intel/oneapi/compiler/2022.2.1/env/vars.sh
$ module load boost/1.81.0
$ tar xzf libint-2.7.2.tar.gz
$ ./autogen.sh
$ CXX=icpc CC=icc ./configure \
  --with-cartgauss-ordering=standard \
  --with-shgauss-ordering=gaussian \
  --with-shell-set=standard \
  --enable-1body=2 \
  --with-max-am=7,7,5 \
  --enable-eri=2 \
  --enable-eri2=2 \
  --enable-eri3=2 \
  --with-eri-max-am=7,7,4 \
  --with-eri2-max-am=7,7,5 \
  --with-eri3-max-am=7,7,5 \
  --disable-eri2-pure-sh \
  --disable-eri3-pure-sh
$ make -j36 export
```

(Copy generated libint-2.7.2.tgz to another location.)

```
$ tar xzf libint-2.7.2.tgz
$ . /apl/psi4/1.7/conda_init.sh
$ cd libint-2.7.2/
$ CXX=icpc CC=icc cmake \
```

```
-DPYTHON_EXECUTABLE=$(which python3) \  
-DCMAKE_INSTALL_PREFIX=/apl/psi4/1.7/libint-2.7.2 \  
-DLIBINT2_PYTHON=ON \  
-DBoost_INCLUDE_DIR=/apl/boost/1.81.0/include \  
-DLIBINT2_SHGAUSS_ORDERING=gaussian \  
.  
$ make -j36  
$ make install
```

psi4

```
#!/bin/sh  
  
# assume miniforge for psi4 was already installed  
  
VERSION=1.7  
INSTALL_PREFIX=/apl/psi4/1.7  
CHEMPS2DIR=/apl/psi4/1.7  
  
BASEDIR=/home/users/${USER}/Software/PSI4/1.7  
TARBALL=${BASEDIR}/psi4.tar.gz  
  
WORKDIR=/gwork/users/${USER}  
PARALLEL=12  
  
#-----  
umask 0022  
export LANG=C  
ulimit -s unlimited  
  
module -s purge  
. ~/intel/oneapi/compiler/2022.2.1/env/vars.sh  
module -s load mkl/2022.2.1  
module -s boost/1.81.0  
  
cd ${WORKDIR}  
if [ -d psi4 ]; then  
  mv psi4 psi4-erase  
  rm -rf psi4-erase &  
fi  
  
# load miniforge3 env  
. ${INSTALL_PREFIX}/conda_init.sh  
  
tar xzf ${TARBALL}  
cd psi4  
  
sed -i -e "s/xHost/march=core-avx2/" cmake/xhost.cmake  
  
mkdir build  
cd build  
cmake .. \  
  -DENABLE_CheMPS2=ON \  
  -DCheMPS2_DIR=${CHEMPS2DIR} \  
  -DMAX_AM_ERI=7 \  
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \  
  -DCMAKE_PREFIX_PATH="/apl/psi4/1.7/libint-2.7.2" \  
  -DLibint2_DIR="/apl/psi4/1.7/libint-2.7.2" \  
  -DBUILD_SHARED_LIBS=ON \  
  -DCMAKE_CXX_COMPILER=icpc \  
  -DCMAKE_C_COMPILER=icc \  
  -DCMAKE_Fortran_COMPILER=ifort  
make -j ${PARALLEL}  
  
make install
```

```
ctest -j${PARALLEL}
```

Notes

- All the psi4 tests passed.
- Automatic build of libint of psi4 does not work. (Errors on Eigen etc.)
 - Built libint-2.7.2 according to the guide in external/upstream/libint2/CMakeLists.txt of PSI4.
 - I'm not sure if this build procedure is really correct. At least all the tests of PSI4 is passed.
 - (Many PSI4 tests output errors when libint was built with other options.)
- GCC build failed with errors related to OpenMP.