# 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 zxf 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 zxf 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 zxf ${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.