

xtb 6.7.0

Webpage

<https://xtb-docs.readthedocs.io/en/latest/>
<https://github.com/grimme-lab/xtb>

Version

6.7.0

Build Environment

- gcc 10.3.1 (gcc-toolset/10)
- Ninja 1.11.1
- Python 3.10 (conda)

Files Required

- xtb and other packages are downloaded in the procedure below.

Build Procedure

```
#!/bin/sh

VERSION=6.7.0
INSTALL_DIR=/apl/xtb/${VERSION}

WORKDIR=/gwork/users/${USER}

XTB_GITHUB=https://github.com/grimme-lab/xtb.git
XTB_TAG=v${VERSION}

# -----

cd ${WORKDIR}
if [ -d ${VERSION} ]; then
  mv ${VERSION} ${VERSION}-remove
  rm -rf ${VERSION}-remove &
fi
git clone ${XTB_GITHUB} ${VERSION}
cd ${VERSION}
git checkout refs/tags/${XTB_TAG}

export OMP_NUM_THREADS=8
./apl/conda/20240305/conda_init.sh

module -s purge
module -s load gcc-toolset/10
module -s load ninja/1.11.1

# install meson
pip3 install --user meson==0.64.1
export PATH=~/local/bin:$PATH

meson setup build \
  --buildtype release \
  --optimization 2 \
  -Dprefix=${INSTALL_DIR} \
  -Dlapack="openblas" \
  -Dopenmp="true"

ninja -C build test
ninja -C build install
```

Tests

One of the tests failed. Changing compiler version or lapack implementation don't help.

- 117/148 xtb:unit / iff FAIL 0.70s exit status 2

Notes

- (assumed to be used with ORCA)
- MKL version also works fine. (We chose OpenBLAS not for performance but for simpler library dependency.)
- Newer version of meson is necessary only in the build stage. We didn't install it to the shared region (like /apl).
 - We didn't test meson version 1.x series.
- New version of GCC (11 or later) failed to build or failed more tests. We thus employ GCC 10 this time.
- GPU utilization is not tested.