

xtb 6.7.1

Webpage

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

Version

6.7.1

Build Environment

- gcc 10.3.1 (gcc-toolset/10)
- Ninja 1.12.1
- Python 3.10 (conda)
- OpenBLAS 0.3.29 (lp64)

Files Required

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

Build Procedure

```
#!/bin/sh

VERSION=6.7.1
INSTALL_DIR=/apl/xtb/${VERSION}

WORKDIR=/gwork/users/${USER}

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

# -----

cd ${WORKDIR}
if [ -d xtb-${VERSION} ]; then
  mv xtb-${VERSION} xtb-${VERSION}-remove
  rm -rf xtb-${VERSION}-remove &
fi
git clone ${XTB_GITHUB} xtb-${VERSION} -b ${XTB_TAG}
cd xtb-${VERSION}

# tblite head -> 0.3.0+ (e5c51c16ad27d348278f8ea8008f608712c545a8)
sed -i -e "s/head/e5c51c16ad27d348278f8ea8008f608712c545a8/" subprojects/tblite.wrap

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

module -s purge
module -s load gcc-toolset/10
module -s load ninja/1.12.1
module -s load openblas/0.3.29-lp64

# 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. (same as 6.7.0 case)

- 106/148 xtb:unit / iff FAIL 0.46s exit status 2

Notes

- GCC 11 and 12 failed to build. GCC 13 can build the executable, but more test failures.
- "head", v0.3.0, v0.4.0 of tblite do not work well (tested on Mar 4, 2025). Slightly old one (not a release version, no tag) was used.