xtb 6.5.1

Webpage

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

Version

6.5.1

Build Environment

- Intel Compiler Classic 2023.2.0
- Intel MKL 2023.2.0
- Ninja 1.11.1
- Python 3.10 (conda)

Files Required

- (none; obtained in the procedure below)

Build Procedure

```
#!/bin/sh

VERSION=6.5.1
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 ${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 ninja/1.11.1

. ~/intel/oneapi/compiler/latest/env/vars.sh # 2023.2.0

module -s load mkl/2023.2.0

export CC=icc
export FC=ifort

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

meson setup build \
        --buildtype release \
        --optimization 2 \
```

```
        -Dprefix=${INSTALL_DIR} \
        -Dla_backend="mkl-static" \
        -Dopenmp="true"

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

Tests

All the tests have passed successfully.

Notes

- xtb 6.6.0 (or later?) has problem with external ORCA (in CENSO). This version is built to work around the problem.
    - ref: https://github.com/grimme-lab/CENSO/issues/50
- When xtb is built with newer version of GCC and used with CENSO 1.2.0, stderr output (e.g. "normal termination of xtb") may appear at a strange place in the output file (confirmed in "ohess.out" file generated during CENSO runs).
    - This results in "ERROR: can not convert G(T)". The calculation does not abort, though.
    - This message might change the computation results (depending on the position where the stderr message is inserted).
    - This problem is not observed when xtb is built with Intel Compiler.