

GENESIS 1.4.0 for LX

Webpage

<https://www.r-ccs.riken.jp/labs/cbrt/>

Version

1.4.0

Build Environment

- Intel Parallel Studio XE 2018 Update 4

Files Required

- genesis-1.4.0.tar.bz2
- tests-1.4.0.tar.bz2

Build Procedure

```
#!/bin/sh

VERSION=1.4.0
BASEDIR=/home/users/${USER}/Software/GENESIS/${VERSION}
SRC_TARBALL=${BASEDIR}/genesis-${VERSION}.tar.bz2
TESTS_TARBALL=${BASEDIR}/tests-${VERSION}.tar.bz2

INSTALLDIR=/local/apl/lx/genesis140

WORKDIR=/work/users/${USER}
BUILDDIR=${WORKDIR}/genesis-${VERSION}
TESTSDIR=${WORKDIR}/tests-${VERSION}

PARALLEL=12
PARALLEL_TESTS=8

# -----
umask 0022

module purge
module load intel_parallelstudio/2018update4

export LANG=C
export LC_ALL=C
export OMP_NUM_THREADS=1

cd ${WORKDIR}
if [ -d genesis-${VERSION} ]; then
  mv genesis-${VERSION} genesis-erase
  rm -rf genesis-erase &
fi

if [ -d tests-${VERSION} ]; then
  mv tests-${VERSION} tests-erase
  rm -rf tests-erase &
fi

tar jxf ${SRC_TARBALL}
tar jxf ${TESTS_TARBALL}

cd ${BUILDDIR}
FC=mpiifort CC=mpiicc ./configure --prefix=${INSTALLDIR}

make depend
```

```
# ad hoc work around; dependency solving script does not take care #include
sed -i -e "/^pr_huge_molecule.o/s$/ pr_huge_molecule_file.o/" src/spdyn/Makefile.depends

make -j ${PARALLEL} && make install

ATDYN=${INSTALLDIR}/bin/atdyn
SPDYN=${INSTALLDIR}/bin/spdyn

cd ${TESTSDIR}/regression_test

# atdyn tests; basic and special one
./test.py      "mpirun -np ${PARALLEL_TESTS} $ATDYN"
./test_vib.py  "mpirun -np ${PARALLEL_TESTS} $ATDYN"

# spdyn tests
./test.py      "mpirun -np ${PARALLEL_TESTS} $SPDYN"
./test_remd.py "mpirun -np ${PARALLEL_TESTS} $SPDYN"
./test_rpath.py "mpirun -np ${PARALLEL_TESTS} $SPDYN"
./test_gamd.py "mpirun -np ${PARALLEL_TESTS} $SPDYN"
```

Notes

- Built and tested on ccfep.
- All the tests were successfully passed.
- QM/MM calculation could run successfully without any critical errors.
 - Official QM/MM tutorial was employed for this test, where Gaussian 16 Rev. C01 was used for the QM/MM calculation.