

GENESIS 1.7.0

ウェブページ

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

バージョン

1.7.0

ビルド環境

- Intel Parallel Studio XE 2018 Update 4

ビルドに必要なファイル

- genesis-1.7.0.tar.bz2
- tests-1.7.0.tar.bz2

ビルド手順

```
#!/bin/sh

VERSION=1.7.0
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/genesis170

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

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 -j ${PARALLEL} && make install
```

```
make && make install
```

```
ATDYN=${INSTALLDIR}/bin/atdyn
```

```
SPDYN=${INSTALLDIR}/bin/spdyn
```

```
cd ${TESTSDIR}/regression_test
```

```
# atdyn tests
```

```
./test.py "mpirun -np ${PARALLEL_TESTS} $ATDYN"
```

```
./test_remd.py "mpirun -np ${PARALLEL_TESTS} $ATDYN"
```

```
./test_rpath.py "mpirun -np ${PARALLEL_TESTS} $ATDYN"
```

```
./test_gamd.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"
```

```
./test_fep.py "mpirun -np ${PARALLEL_TESTS} $SPDYN"
```

```
cd test_analysis
```

```
./test_analysis.py ${INSTALLDIR}/bin
```

```
cd ../
```

```
cd test_spana
```

```
./test_spana.py ${INSTALLDIR}/bin
```

```
cd ..
```

メモ

- テストはすべて通過
- intel2020u2 ではテスト途中で停止するため回避
- 並列 make は正しく動作せず