

GENESIS 1.7.0 with GPU support

Webpage

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

Version

1.7.0

Build Environment

- Intel Parallel Studio XE 2018 Update 4
- CUDA 11.1 Update 1

Files Required

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

Build Procedure

```
#!/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-CUDA

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

PARALLEL_TESTS=8

# -----
umask 0022

module purge
module load intel_parallelstudio/2018update4
module load cuda/11.1

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} \
```

```
--enable-gpu \  
--enable-single \  
--with-cuda=/local/apl/lx/cuda-11.1
```

```
make && make install
```

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

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

```
# spdyn tests
```

```
./test.py "mpirun -np ${PARALLEL_TESTS} $SPDYN" gpu  
./test_remd.py "mpirun -np ${PARALLEL_TESTS} $SPDYN" gpu  
./test_rpath.py "mpirun -np ${PARALLEL_TESTS} $SPDYN" gpu  
./test_gamd.py "mpirun -np ${PARALLEL_TESTS} $SPDYN" gpu  
./test_fep.py "mpirun -np ${PARALLEL_TESTS} $SPDYN" gpu
```

Notes

- All the tests has passed. (excluding nine "cutoff" system tests of test_remd.)
- Spdyn binary will run both on P100 and V100. (Compute capabilities corresponding to them might not be explicitly specified, though.)
- cuda-11.4 (compatibility mode) version does not work properly due to the unknown reason.