

GENESIS 2.1.2 with GPU support

Webpage

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

Version

2.1.2

Build Environment

- gcc 12.1.1 (gcc-toolset/12)
- MKL 2024.0
- Open MPI 4.1.6
- CUDA 12.1 Update 1

Files Required

- genesis-2.1.2.tar.bz2
- tests-2.1.2.tar.bz2

Build Procedure

Submitted with this job script.

```
#!/bin/sh
#PBS -l select=1:ncpus=8:mpiprocs=8:ompthreads=1:ngpus=1
#PBS -l walltime=24:00:00

cd $PBS_O_WORKDIR

VERSION=2.1.2
BASEDIR=/home/users/${USER}/Software/GENESIS/${VERSION}
SRC_TARBALL=${BASEDIR}/genesis-${VERSION}.tar.bz2
TESTS_TARBALL=${BASEDIR}/tests-${VERSION}.tar.bz2

INSTALLDIR=/apl/genesis/2.1.2-CUDA

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

PARALLEL_TESTS=8

# -----
umask 0022

module -s purge
module -s load gcc-toolset/12
module -s load mkl/2024.0
module -s load openmpi/4.1.6/gcc12
module -s load cuda/12.1u1

export LANG=C
export LC_ALL=C
export OMP_NUM_THREADS=1
ulimit -s unlimited

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 ${BUILDDIR}
FC=mpif90 CC=mpicc \
LAPACK_LIBS="-L${MKLRROOT}/lib/intel64 -WI,--no-as-needed -lmkl_gf_lp64 -lmkl_gnu_thread -lmkl_core -lgomp -lpthread -lm -ldl" \
./configure --prefix=${INSTALLDIR} \
  --enable-gpu \
  --enable-single \
  --with-cuda=/opt/cuda/12.1.1

make && make install

SPDYN=${INSTALLDIR}/bin/spdyn

cd ${TESTSDIR}/regression_test

for f in test.py test_remd.py test_fep.py test_rpath.py \
  test_gamd.py; do
  sed -i -e "s/env python/env python3/" $f
done

# 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"

```

Notes

- If hardware specification for A100 (-gencode for compute capability 8.0) was added, compilation failed.