

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

1.6.0

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

- genesis-1.6.0.tar.bz2
- tests-1.6.0.tar.bz2
- fortdep.py.patch

```
--- fortdep.py.org 2020-12-28 14:05:33.000000000 +0900
+++ fortdep.py 2020-12-28 14:39:43.000000000 +0900
@@ -24,6 +24,7 @@
     re_fcomment = re.compile( "(^[^!]*)(.*$)" )
     re_module = re.compile( "^(.*;+|s*)\s*module\s*([^\s,]*)\s*", re.I )
     re_use = re.compile( "^(.*;+|s*)\s*use\s+([^\s,]*)\s*", re.I )
+ re_include = re.compile( "^(\\s*)#include\s+[\"']([^\"]+)[\"']\s*" )
     mod_ext = ".mod"

     def __init__( self, fname = "", ext = ".o" ):
@@ -31,6 +32,7 @@
         self.filename = fname
         self.modules = []
         self.depmods = []
+ self.includes = []

     def setFilename( self, fname, ext = ".o" ):
         if len(fname) == 0:
@@ -54,6 +56,14 @@
         if ( ma ):
             modname = ma.group(2).lower()
             self.appendDependMods( modname )
+ mi = FortranFile.re_include.search( line )
+ if ( mi ):
+     srcname = mi.group(2)
+     if re.search( r".h$", srcname, re.I ):
+         #self.includes.append( srcname )
+         pass
+     else:
+         self.includes.append( re.sub( r"\.[a-zA-Z0-9]+$", ".o", srcname ) )
         myf.close()
         self.makeUniqList()

@@ -64,8 +74,9 @@
         self.depmods.append( modname + FortranFile.mod_ext )

     def makeUniqList( self ):
- self.modules = list(set(self.modules))
- self.depmods = list(set(self.depmods))
+ self.modules = list(set(self.modules))
+ self.depmods = list(set(self.depmods))
+ self.includes = list(set(self.includes))

     def getMyModuleFileNames( self ):
```

```

return self.modules
@@ -87,7 +98,8 @@
    if m.lower() in mods_avail or not mods_avail:
        depmods.append(m)
    ret = ""
-   ret += self.objname + ": " + self.filename + " " + ".join(depmods) + " " + static_deps
+   ret += self.objname + ": " + self.filename + " " + ".join(depmods) + \
+       " " + ".join(self.includes) + " " + static_deps
    if len(self.modules) > 0:
        ret += "\n"
    ret += ".join(self.modules) + ": " + self.filename + " " + self.objname

```

Build Procedure

```

#!/bin/sh

VERSION=1.6.0
BASEDIR=/home/users/${USER}/Software/GENESIS/${VERSION}
SRC_TARBALL=${BASEDIR}/genesis-${VERSION}.tar.bz2
TESTS_TARBALL=${BASEDIR}/tests-${VERSION}.tar.bz2
FORTDEP_PATCH=${BASEDIR}/fortdep.py.patch

INSTALLDIR=/local/apl/lx/genesis160-CUDA

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
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}
patch -p0 < ${FORTDEP_PATCH}
FC=mpiifort CC=mpiicc ./configure --prefix=${INSTALLDIR} \
    --enable-gpu \
    --enable-single \
    --with-cuda=/local/apl/lx/cuda-11.1
make depend

make -j ${PARALLEL} && 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 can run both on P100 and V100. (Compute capabilities corresponding to them might not be explicitly specified, though.)