

CASTEP 16.1 Installation Best Practices

1. Introduction:

The following best practices document is provided as courtesy of the HPC Advisory Council.

2. Application Description:

CASTEP is a commercial software package which uses density functional theory with a plane wave basis set to calculate the electronic properties of crystalline solids, surfaces, molecules, liquids and amorphous materials from first principles. The abbreviation stands for Cambridge Serial Total Energy Package

3. Version Information:

CASTEP 16.1. More information about CASTEP is available at <http://www.castep.org/>.

4. Prerequisites:

The instructions from this best practice have been tested on the following configuration:

Hardware:

- Dell PowerEdge R730 32-node (1024-core) "Thor" cluster.
- Dual-Socket 14-Core Intel E5-2697A v4 @ 2.60 GHz CPUs
- Mellanox ConnectX-4 EDR InfiniBand adapters
- Mellanox Switch-IB SB7700 VPI InfiniBand switch

OS and software:

- RHEL 7.2
- MLNX_OFED_LINUX-3.3-1.0.4.0 InfiniBand SW stack
- MPI: [Mellanox HPC-X v1.7.402](#) and Intel MPI 5.1.3
- Compilers: Intel 2016.4.258

5. Building Sources

5.1 Building HPC-X

The following shows the steps to compile CASTEP using Mellanox HPC-XMPI toolkit. We want to recompile HPC-X in order to advantage of better support with the latest Intel compilers

```
#!/bin/bash
module purge
module load intel/compiler/2016.4.258

export CC=icc
export CXX=icpc
export FC=ifort
export F77=ifort

rm -rf /dev/shm/openmpi-gitclone
tar xfp openmpi-gitclone.tar.gz -C /dev/shm
cd /dev/shm/openmpi-gitclone
```

```

module use /opt/hpcx-v1.7.402-icc-MLNX_OFED_LINUX-3.3-1.0.0.0-redhat7.2-x86_64/
modulefiles
module load hpcx

./configure --prefix=${HPCX_HOME}/mpi-v1.10.i2016 --with-knem=${HPCX_HOME}/knem \
m \
    --with-fca=${HPCX_HOME}/fca --with-mxm=${HPCX_HOME}/mxm \
    --with-hcoll=${HPCX_HOME}/hcoll \
    --with-platform=contrib/platform/mellanox/optimized \
    --with-slurm --with-pmi \
    --with-verbs 2>&1 | tee config-output.log

#         --enable-mpi-thread-multiple

make -j32 all 2>&1 |tee build.log
make -j24 install 2>&1| tee install.log

cd /opt/hpcx-v1.7.402-icc-MLNX_OFED_LINUX-3.2-2.0.0.0-redhat7.2-x86_64/modulefiles
sed -e 's#mpi-v1.10#mpi-v1.10.i2016#' hpcx-mpi-v1.10 > hpcx.i2016a

```

5.2 Building CASTEP

The following shows the steps to compile CASTEP using Mellanox HPC-XMPI Toolkit that is based on Open MPI. The same procedure can apply for building with Intel MPI.

```

module load intel/compiler/2016.4.258
export CASTEP_ARCH=linux_x86_64_ifort15
make clean
make COMMS_ARCH=mpi FFT=mk1 MATHLIBS=mk110 -j 32
make install

```

6. Running CASTEP

6.1 Running CASTEP using Mellanox HPC-X

The following shows the runtime parameter used for running CASTEP using Mellanox HPC-XMPI Toolkit:

```

module load intel/compiler/2016.4.258
module use /opt/hpcx-v1.7.402-icc-MLNX_OFED_LINUX-3.3-1.0.0.0-redhat7.2-x86_64/
modulefiles
module load hpcx

mpirun -np 256 -bind-to core -mca btl_sm_use_knem 1 -mca coll_fca_enable 0 -mca
coll_hcoll_enable 1 -mca coll_hcoll_np 0 -x HCOLL_ENABLE_MCAST_ALL=1 -x HCOLL_
CONTEXT_CACHE_ENABLE=1 -mca pml yalla -mca mtl_mxm_np 0 -x MXM_TLS=ud,shm,self
-x MXM_RDMA_PORTS=mlx5_0:1 -mca btl_openib_if_include mlx5_0:1 --mca mpi_leave_
pinned 1 -x MALLOC_MMAP_MAX=0 -x MALLOC_TRIM_THRESHOLD=-1 -x HCOLL_ML_DISABLE

```

```
_ALLTOALLV=1 -mca coll_tuned_use_dynamic_rules 1 -mca coll_tuned_alltoallv_algo  
rithm 1 /home/castep/CASTEP-v16.1.hg-hpcx-test/obj/linux_x86_64_ifort15/castep.  
mpi hamilton7
```

6.2 Running CASTEP using Intel MPI

The following shows the runtime parameter used for running CASTEP using Intel MPI:

```
module load intel/compiler/2016.4.258  
module load intel/impi/5.1.3.258  
  
mpirun -np 256 -genv I_MPI_PIN on -genv I_MPI_DEBUG 4 -genv DAT_OVERRIDE /etc/d  
at.conf -genv I_MPI_DAT_LIBRARY /usr/lib64/libdat2.so -DAPL -genv I_MPI_FABRICS  
shm:dapl -genv I_MPI_DAPL_UD enable -genv I_MPI_DAPL_PROVIDER ofa-v2-m1x5_0-1u  
-genv DAPL_MAX_INLINE 256 -genv I_MPI_DAPL_RDMA_RNDV_WRITE on -genv DAPL_IB_MT  
U 4096 -genv I_MPI_PIN_DOMAIN socket -genv I_MPI_ADJUST_ALLREDUCE=4 -genv I_MPI  
_ADJUST_ALLTOALLV=1 -genv I_MPI_STATS=all /home/castep/CASTEP-v16.1.hg-impi/bin  
/linux_x86_64_ifort16/castep.mpi hamilton7
```